DISLOCATION PROBLEMS FOR PERIODIC SCHröDINGER OPERATORS AND MATHEMATICAL ASPECTS OF SMALL ANGLE GRAIN BOUNDARIES

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ABSTRACT. We discuss two types of defects in two-dimensional lattices, namely (1) translational dislocations and (2) defects produced by a rotation of the lattice in a half-space.

For Lipschitz-continuous and \( \mathbb{Z}^2 \)-periodic potentials, we first show that translational dislocations produce spectrum inside the gaps of the periodic problem; we also give estimates for the (integrated) density of the associated surface states. We then study lattices with a small angle defect where we find that the gaps of the periodic problem fill with spectrum as the defect angle goes to zero. To introduce our methods, we begin with the study of dislocation problems on the real line and on an infinite strip. Finally, we consider examples of muffin tin type. Our overview refers to results in [HK1, HK2].

1. INTRODUCTION

In solid state physics, pure matter in a crystallized form is usually described by a periodic Schrödinger operator \(-\Delta + V(x)\) in \(\mathbb{R}^3\), where the potential \(V\) is a periodic function. In reality, however, crystals are not perfectly periodic since the periodic pattern of atomic arrangement is disturbed by various types of crystal defects, most notably:

— point defects where single atoms are removed (vacancies) or replaced by foreign atoms (impurities),
— large scale defects that produce a surface at which two portions of the lattice (or two different half-lattices) face each other (line defects, grain boundaries).

For the modeling of point defects, random Schrödinger operators are the appropriate setting (cf., e.g., [PF] or [V]). Here we present a deterministic approach to some two-dimensional models with defects from the second class.

Let \(V : \mathbb{R}^2 \to \mathbb{R}\) be (bounded and) periodic with respect to the lattice \(\mathbb{Z}^2\) and consider the family of potentials

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

(1.1)

We then let \(D_t := -\Delta + W_t\) denote the associated (self-adjoint) Schrödinger operators, acting in \(L_2(\mathbb{R}^2)\). The operators \(D_t\) are the Hamiltonians for a two-dimensional lattice where the potential equals the \(\mathbb{Z}^2\)-periodic function \(V\) on \(\{x \geq 0\}\) and a shifted copy of \(V\) for \(\{x < 0\}\), i.e., we study a dislocation problem. We call \(W_t\) the dislocation potential, \(t\) the dislocation parameter and \(D_t\) the dislocation operators.
The spectrum of $D_0 = D_1$ is purely absolutely continuous and has a band-gap structure,
\[
\sigma(D_0) = \sigma_{\text{ess}}(D_0) = \bigcup_{k=1}^{\infty} [a_k, b_k], \quad a_k < b_k \leq a_{k+1}.
\] (1.2)
The spectral gaps $(b_k, a_{k+1})$ are denoted as $\Gamma_k$. For simplicity, we will sometimes write $a$ and $b$ for the edges of a given $\Gamma_k$ with $\Gamma_k \neq \emptyset$. We shall say that a gap $\Gamma_k = (a, b)$ is non-trivial if $a < b$ and $a$ is above the infimum of the essential spectrum of the given self-adjoint operator.

We will show that the operators $D_t$ possess surface states (i.e., spectrum produced by the interface) in the gaps $\Gamma_k$ of $D_0$, for suitable values of $t \in (0, 1)$. More strongly, we have a positivity result for the (integrated) density of the surface states associated with the above spectrum in the gaps. Here we first have to choose an appropriate scaling which permits to distinguish the bulk from the surface density of states. To this end, 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 limit $n \to \infty$ (which exists as explained in [KS, 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 $\mathcal{J} \subset \mathbb{R} \setminus \sigma(D_0)$. (The fact that an integrated surface density of states exists does not necessarily mean it is non-zero and there are only rare examples where we know $\rho_{\text{surf}}$ to be non-trivial.) Our first main result can be described as follows:

1.1. Theorem. If $(a, b)$ is a non-trivial spectral gap of the periodic operator $-\Delta + V$, acting in $L_2(\mathbb{R}^2)$ with $V$ Lipschitz-continuous, then for any interval $(\alpha, \beta)$ with $a < \alpha < \beta < b$ there is a $t \in (0, 1)$ such that $\rho_{\text{surf}}(D_t, (\alpha, \beta)) > 0$.

We also explain how to obtain upper bounds (as in [HK2]) for the surface density of states. In Section 2, we will outline a proof of Theorem 1.1 starting from dislocation problems on $\mathbb{R}$ and on the strip $\Sigma := \mathbb{R} \times [0, 1]$. The one-dimensional dislocation problem has been studied extensively by Korotyaev [K1, K2], and we use the 1D model mainly for testing our methods in the simplest possible case.

The techniques and results connected with Theorem 1.1 are mainly presented as a preparation for the study of rotational defects where we consider the potential
\[
V_\vartheta(x, y) := \begin{cases} 
V(x, y), & x \geq 0, \\
V(M_{-\vartheta}(x, y)), & x < 0,
\end{cases}
\] (1.3)
where $M_\vartheta \in \mathbb{R}^{2 \times 2}$ is the usual orthogonal matrix associated with rotation through the angle $\vartheta$. The self-adjoint operators $R_\vartheta := -\Delta + V_\vartheta$ in $L_2(\mathbb{R}^2)$ are the Hamiltonians for two half-lattices given by the potential $V$ in $\{x \geq 0\}$ and a rotated copy of $V$ for $\{x < 0\}$; we obtain an interface at $x = 0$ where the two copies meet under the defect angle $\vartheta$. Our main assumption is that the periodic operator $H := R_0$ has a non-trivial gap $(a, b)$. We then have $R_\vartheta \to R_{\vartheta_0}$ in the strong resolvent sense as $\vartheta \to \vartheta_0 \in [0, \pi/2]$; in particular $R_\vartheta$ converges to $H$ in the strong resolvent sense as $\vartheta \to 0$. Our main result, Theorem 1.2 below, shows that the spectrum of $R_\vartheta$ is discontinuous at $\vartheta = 0$; in particular, $R_\vartheta$ cannot converge to $H$ in the norm resolvent sense as $\vartheta \to 0$. 
1.2. Theorem. Let $H$, $R_0$ and $(a,b)$ as above with a Lipschitz-continuous potential $V$. Then, for any $\epsilon > 0$, there exists $0 < \vartheta < \pi/2$ such that for any $E \in (a,b)$ we have

$$\sigma(R_0) \cap (E - \epsilon, E + \epsilon) \neq \emptyset, \quad \forall 0 < \vartheta < \vartheta_\epsilon. \quad (1.4)$$

As an illustration, we will consider potentials of muffin tin type which can be specified by fixing a radius $0 < r < 1/2$ for the discs where the potential vanishes, and the center $P_0 = (x_0, y_0) \in [0,1]^2$ for the generic disc. In other words, we consider the periodic sets

$$\Omega_{r,P_0} := \cup_{(i,j) \in \mathbb{Z}^2} B_r(P_0 + (i,j)), \quad (1.5)$$

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 $H_{i,j}$ 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 $\oplus_{(i,j) \in \mathbb{Z}^2} H_{i,j}$. In our examples, we can see the behavior of surface states in the dislocation problem and the rotation problem for $-\Delta + V_{r,P_0}$ directly.

The paper is organized as follows: Section 2 is devoted to the dislocation problem on $\mathbb{R}$, on $\Sigma$ and in $\mathbb{R}^2$. Section 3 is about a small angle defect model in 2D and explains some details of the proof of Theorem 1.2. Finally, in Section 4, we turn to dislocations and rotations for muffin tin potentials where results analogous to Theorem 1.1 and Theorem 1.2 can be obtained. For further reading, we refer to [HK1, HK2].

2. Dislocation problems on the real line, on the strip $\mathbb{R} \times [0,1]$, and in the plane

In this section, we study Schrödinger operators in one and two dimensions where the potential is obtained from a periodic potential by a coordinate shift on $\{x < 0\}$. We begin with a brief overview of the one-dimensional dislocation problem. In a second step, we study the dislocation problem on the strip $\Sigma = \mathbb{R} \times [0,1]$ which provides a connection between the dislocation problems in one and two dimensions. Finally, we deal with dislocations in $\mathbb{R}^2$. Some of the results obtained in this section will be used in our treatment of rotational defects in the following section.

Let $h_0$ denote the (unique) self-adjoint extension of $-\Delta_{\mathbb{R}^d}$ defined on $C^\infty_c(\mathbb{R})$. Our basic class of potentials is given by

$$P := \{ V \in L^1_{\text{loc}}(\mathbb{R},\mathbb{R}) \mid \forall x \in \mathbb{R} : V(x+1) = V(x) \}.$$ \hspace{1cm} (2.1)

Potentials $V \in P$ belong to the class $L^1_{\text{loc}, \text{unif}}(\mathbb{R})$ 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 $V \in P$ and $t \in [0,1]$, we define the dislocation potentials $W_t$ by $W_t(x) := V(x)$, for $x \geq 0$, and $W_t(x) := V(x + t)$, for $x < 0$. 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

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

where the numbers $\gamma_k$ 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 \( \gamma_{k+1} > \gamma_k' \).

It is easy to see ([HK1]) that
\[
\sigma_{\text{ess}}(H_t) = \sigma_{\text{ess}}(H), \quad 0 \leq t \leq 1,
\]

(2.3)
since inserting a Dirichlet boundary condition at a finite number of points means a finite rank perturbation of the resolvent, as is well known. Hence each non-trivial gap \((a, b)\) of \( H \) is a gap in the essential spectrum of \( H_t \), for all \( t \). However, the dislocation may produce discrete (and simple) eigenvalues inside the spectral gaps of \( H \): for any \((a, b)\) with \( \inf \sigma_{\text{ess}}(H) < a < b \) and \((a, b) \cap \sigma(H) = \emptyset\) there exists \( t \in (0, 1) \) such that
\[
\sigma(H_t) \cap (a, b) \neq \emptyset.
\]

(2.4)
We thus have the following picture: while the essential spectrum remains unchanged under the perturbation, eigenvalues of \( H_t \) cross the (non-trivial) gaps of \( H \) as \( t \) ranges through \((0, 1)\). These eigenvalues of \( H_t \) can be described by continuous functions of \( t \) (cf. [K1, K2] and Lemma 2.1 below). Lemma 2.1 states the (more or less obvious) fact that the 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 \([0, 1]\). The proof of Lemma 2.1 uses a straightforward compactness argument (cf. [HK1]). The result stated in Lemma 2.1 is presumably far from optimal if one assumes periodicity of the potential. On the other hand, the lemma and its proof in [HK1] allow for a generalization to non-periodic situations.

2.1. Lemma. Let \( V \in \mathcal{P} \) and \( k \in \mathbb{N} \) and suppose that the gap \( \Gamma_k \) of \( H \) is open. 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) For all \( j \) and for all \( \alpha_j < t < \beta_j \), \( f_j(t) \) is an eigenvalue of \( H_t \). Conversely, for any \( t \in (0, 1) \) and any eigenvalue \( \hat{E} \in \Gamma_k \) of \( H_t \) there is a unique index \( j \) such that \( f_j(t) = \hat{E} \).

(ii) As \( t \downarrow \alpha_j \) (or \( t \uparrow \beta_j \)), the limit of \( f_j(t) \) exists and belongs to the set \( \{a, b, \} \).

(iii) For all but a finite number of indices \( j \) the range of \( f_j \) does not intersect a given compact subinterval of \( \Gamma_k \).

Under stronger assumptions on \( V \) one can show that the eigenvalue branches are Hölder- or Lipschitz-continuous, or even analytic (cf. [K1]): we consider potentials from the classes
\[
\mathcal{P}_\alpha := \left\{ V \in \mathcal{P} \mid \exists C \geq 0: \int_0^1 |V(x + s) - V(x)| \, dx \leq Cs^\alpha, \forall 0 < s \leq 1 \right\},
\]

(2.5)
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. As shown by J. Voigt, \( \mathcal{P}_1 \) coincides with the class of periodic functions on the real line which are locally of bounded variation (cf. [HK1]).

2.2. Proposition. For \( V \in \mathcal{P}_1 \), let \( (a, b) \) denote any of the gaps \( \Gamma_k \) of \( H \) and let \( f_j : (\alpha_j, \beta_j) \to (a, b) \) be as in Lemma 2.1. Then the functions \( f_j \) are uniformly
Lipschitz-continuous. More precisely, there exists a constant $C \geq 0$ such that for all $j$
\begin{equation}
|f_j(t) - f_j(t')| \leq C|t - t'|, \quad \alpha_j \leq t, t' \leq \beta_j.
\end{equation}

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, 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 $t, t' \in [\alpha'_j, \beta'_j]$.

Our basic result in the study of the one-dimensional dislocation problem says 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 $f_i(\alpha_i) := \lim_{t \uparrow \alpha} f_i(t), \quad f_i(\beta_i) := \lim_{t \downarrow \beta} f_i(t)$, we define
\begin{equation}
N_k := \# \{ i \mid f_i(\alpha_i) = b, \quad f_i(\beta_i) = a \} - \# \{ i \mid f_i(\alpha_i) = a, \quad f_i(\beta_i) = b \}
\end{equation}
(note that both terms on the RHS of eqn. (2.7) are finite by Lemma 2.1 (iii)). Thus $N_k$ 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, $N_k$ is the spectral multiplicity which effectively crosses the gap $\Gamma_k$ in downwards direction as $t$ increases from 0 to 1. We then have the following result.

2.3. Theorem. (cf. [K1, HK1])

Let $V \in \mathcal{P}$ and let $k \in \mathbb{N}$ be such that the $k$-th spectral gap of $H$ is open, i.e., $\gamma'_k < \gamma_{k+1}$. Then $N_k = k$.

In fact, the results obtained by Korotyaev in [K1, K2] are more detailed; e.g., Korotyaev shows that the dislocation operator produces at most two states (an eigenvalue and a resonance) in a gap of the periodic problem. On the other hand, our variational arguments are more flexible and allow an extension to higher dimensions, as we will see in the sequel. The main idea of our proof—somewhat reminiscent of [DH, ADH]—goes as follows: consider a sequence of approximations on intervals $(-n - t, n)$ with associated operators $H_{n,t} = -\frac{d^2}{dx^2} + W_t$ with periodic boundary conditions. We first observe that the gap $\Gamma_k$ is free of eigenvalues of $H_{n,0}$ and $H_{n,1}$ since both operators are obtained by restricting a periodic operator on the real line to some interval of length equal to an entire multiple of the period, with periodic boundary conditions. Second, the operators $H_{n,t}$ have purely discrete spectrum and it follows from Floquet theory (cf. [E, RS-IV]) that $H_{n,0}$ has precisely $2n$ eigenvalues in each band while $H_{n,1}$ has precisely $2n + 1$ eigenvalues in each band. As a consequence, effectively $k$ eigenvalues of $H_{n,t}$ must cross any fixed $E \in \Gamma_k$ as $t$ increases from 0 to 1. To obtain the result of Theorem 2.3 we only have to take the limit $n \to \infty$; cf. [HK1] for the technical arguments. In [HK1], we also discuss a one-dimensional periodic step potential and perform some explicit (and also numerical) computations resulting in a plot of an eigenvalue branch for the associated dislocation problem.

We now turn to the dislocation problem on the infinite strip $\Sigma = \mathbb{R} \times [0, 1]$. Let $V : \mathbb{R}^2 \to \mathbb{R}$ be $\mathbb{Z}^2$-periodic and Lipschitz continuous. 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. (1.1); 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. To see 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 \( t \in [0, 1] \), it suffices to prove compactness of the resolvent difference \((S_t - c)^{-1} - (S_{t,D} - c)^{-1}\), 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 band gap structure of the essential spectrum of \( S_t \) is independent of \( t \in [0, 1] \), \( S_t \) will have discrete eigenvalues in the spectral gaps of \( S_0 \) for appropriate values of \( t \). We have the following result.

### 2.4. Theorem

Assume that \( V \) is Lipschitz-continuous. Let \((a, b)\) denote a non-trivial spectral gap of \( S_0 \) and let \( E \in (a, b) \). Then there exists \( t = t_E \in (0, 1) \) such that \( E \) is a discrete eigenvalue of \( S_t \).

As on the real line, we work with approximating problems on finite size sections of the infinite strip \( \Sigma \). Let \( \Sigma_{n,t} := (-n - t, n) \times (0, 1) \) for \( n \in \mathbb{N} \), 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. Thus for any \( n \in \mathbb{N} \) we can find \( t_n \in (0, 1) \) such that \( E \in \sigma_{\text{disc}}(S_{n,t_n}) \); furthermore, there are eigenfunctions \( u_n \in D(S_{n,t_n}) \) satisfying \( S_{n,t_n} u_n = \lambda u_n \), \( \|u_n\| = 1 \), and \( \|\nabla u_n\| \leq C \) for some constant \( C \geq 0 \). Multiplying \( u_n \) with a suitable cut-off function, we obtain (after extracting a suitable subsequence) functions \( v_n \in D(S_t) \) and \( t \in (0, 1) \) satisfying

\[
\|(S_t - E)v_n\| \to 0 \quad \text{and} \quad |v_n| \to 1, \tag{2.8}
\]

as \( n \to \infty \), which implies \( E \in \sigma(S_t) \), cf. [HK1].

Finally, we consider the dislocation problem on the plane \( \mathbb{R}^2 \) where we study the operators

\[
D_t = -\Delta + W_t, \quad 0 \leq t \leq 1. \tag{2.9}
\]

Denote by \( S_t(\theta) \) the operator \( S_t \) on the strip \( \Sigma \) with \( \theta \)-periodic boundary conditions in the \( y \)-variable. Since \( W_t \) is periodic with respect to \( y \), we have

\[
D_t \simeq \int_{[0,2\pi]} S_t(\theta) \frac{d\theta}{2\pi}; \tag{2.10}
\]

in particular, \( D_t \) has no singular continuous part, cf. [DS]. As for the spectrum of \( S_t \) inside the gaps of \( S_0 \), Theorem 2.4 yields the following result.
2.5. Theorem. Assume that $V$ is Lipschitz-continuous. Let $(a, b)$ denote a non-trivial spectral gap of $D_0$ and let $E \in (a, b)$. Then there exists $t = t_E \in (0, 1)$ with $E \in \sigma(D_t)$.

Proof. Let $v_n \in D(S_t)$ denote an approximate solution of the eigenvalue problem for $S_t$ and $E$; see (2.8). We extend $v_n$ to a function $\tilde{v}_n(x, y)$ on $\mathbb{R}^2$ which is periodic in $y$. By multiplying $\tilde{v}_n$ by smooth cut-off functions $\Phi_n(x, y)$, we obtain functions $w_n = w_n(x, y) := \frac{1}{\|\Phi_n \tilde{v}_n\|} \Phi_n \tilde{v}_n \quad (2.11)$ belonging to the domain of $D_t$ and satisfying $\|w_n\| = 1$, supp $w_n \subset [-n, n]^2$, and $(D_t - E)w_n \to 0, \quad n \to \infty; \quad (2.12)$ this implies the desired result. \qed

The stronger statement in Theorem 1.1. follows by a very similar line of argument. The upshot is that the dislocation moves enough states through the gap to have a non-trivial (integrated) surface density of states, for suitable parameters $t$.

The lower estimate established in Theorem 1.1. is complemented by an upper bound which is of the expected order (up to a logarithmic factor) in [HK2]. Note that the situation treated in [HK2] is far more general than the rotation or dislocation problems studied so far. In fact, here we allow for different potentials $V_1$ on the left and $V_2$ on the right which are only linked by the assumption that there is a common spectral gap; neither $V_1$ nor $V_2$ are required to be periodic. The proof uses technology which is fairly standard and is based on exponential decay estimates for resolvents, cf. [S].

2.6. Theorem. Let $V_1, V_2 \in L_\infty(\mathbb{R}^2, \mathbb{R})$ and suppose that the interval $(a, b) \subset \mathbb{R}$ does not intersect the spectra of the self-adjoint operators $H_k := -\Delta + V_k$, $k = 1, 2$, both acting in the Hilbert space $L_2(\mathbb{R}^2)$. Let $W := \chi_{\{x < 0\}} \cdot V_1 + \chi_{\{x \geq 0\}} \cdot V_2 \quad (2.13)$ and define $H := -\Delta + W$, a self-adjoint operator in $L_2(\mathbb{R}^2)$. Finally, we let $H^{(n)}$ denote the self-adjoint operator $-\Delta + W$ acting in $L_2(Q_n)$ with Dirichlet boundary conditions. Then, for any interval $[a', b'] \subset (a, b)$, we have

$$\limsup_{n \to \infty} \frac{1}{n \log n} N_{[a', b']}(H^{(n)}) < \infty, \quad (2.14)$$

where $N_{[a', b']}(H^{(n)})$ denotes the number of eigenvalues of $H^{(n)}$ in $[a', b']$.

We note that the factor $\log n$ in eqn. (2.14) can presumably be dropped under appropriate assumptions (H. Cornean, private communication); however, this seems to require substantially different, and less elementary, methods.

3. Rotational defect in a two-dimensional lattice

In this section, we will use our results on the translational problem to obtain spectral information about rotational problems in the limit of small angles. Our
main theorem deals with the following situation. Let \( V : \mathbb{R}^2 \to \mathbb{R} \) be a Lipschitz-continuous function which is periodic w.r.t. the lattice \( \mathbb{Z}^2 \). For \( \vartheta \in (0, \pi/2) \), let

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

and \( V_\vartheta \) as in (1.3). We then let \( H_0 \) denote the (unique) self-adjoint extension of \( -\Delta \mid C_c^\infty(\mathbb{R}^2) \), acting in the Hilbert space \( L_2(\mathbb{R}^2) \), and

\[
R_\vartheta := H_0 + V_\vartheta, \quad D(R_\vartheta) = D(H_0).
\]

Then \( R_\vartheta \) is essentially self-adjoint on \( C_c^\infty(\mathbb{R}^2) \) and semi-bounded from below.

Now our key observation consists in the following: for any \( t \in (0, 1) \) given, any \( \varepsilon > 0 \), and any \( n \in \mathbb{N} \), we can find points \((0, \eta)\) on the \( y\)-axis with \( \eta \in \mathbb{N} \) such that

\[
|V_\vartheta(x, y) - W_t(x, y)| < \varepsilon, \quad (x, y) \in Q_n(0, \eta),
\]

where \( Q_n(0, \eta) = (-n, n) \times (\eta - n, \eta + n) \), provided \( \vartheta > 0 \) is small enough and satisfies a condition which ensures an appropriate alignment of the period cells on the \( y\)-axis. Put differently: for very small angles, the rotated potential \( V_\vartheta \) will almost look like a dislocation potential \( W_t \), on suitable squares \( Q_n(0, \eta) \).

To prove Theorem 1.2 we proceed as follows: Fix an arbitrary \( \Theta \subset \mathbb{T}^2 \) as defined by

\[
T_\vartheta(x, y) := (x + \tan \vartheta, y + 1/\cos \vartheta).
\]

Then there is a set \( \Theta \subset (0, \pi/2) \) with countable complement such that the transformation \( T_\vartheta \) in (3.5) is ergodic for all \( \vartheta \in \Theta \).

The assertion of Theorem 1.2 now follows from Birkhoff’s ergodic theorem, cf. [CFS, HK2]: Let us first assume that \( \vartheta \in \Theta \). Let \( \varepsilon > 0 \) and let us denote by \( \chi = \chi_Q \) the characteristic function of the set \( Q := (t - \varepsilon, t + \varepsilon) \times (-\varepsilon, \varepsilon) \subset \mathbb{T}^2 \). Then

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{m=0}^{n-1} \chi(T_\vartheta^m(0, 0)) = \int_Q \, dx \, dy = 4\varepsilon^2 > 0.
\]

By a simple approximation argument the statement of Theorem 1.2 also holds for angles \( \vartheta \notin \Theta \). Altogether, this completes the proof of Theorem 1.2.

Recall that strong resolvent convergence implies upper semi-continuity of the spectrum while the spectrum may contract considerably when the limit is reached. In the present section, we are dealing with a situation where the spectrum in fact behaves discontinuously at \( \vartheta = 0 \) since, counter to first intuition, the spectrum of
In this section, we present a class of examples where one can arrive at rather precise statements that illustrate some of the phenomena described before. Our potentials $V = V_{r, R}$ are of muffin tin type, as defined in the introduction.

(1) The dislocation problem. In the simplest case we would take $x_0 = 1/2$ and $y_0 = 0$ so that the disks $B_r(1/2 + i, j)$, for $i, j \in \mathbb{Z}$, will not intersect or touch the interface $\{(x, y) \mid x = 0\}$, for $0 < r < 1/2$. Defining the dislocation potential $W_i$ as in (1.1), 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 $B_r(1/2 - t, 0) \cap \{x < 0\}$, for $1/2 - r < t < 1/2 + r$, are denoted as $\lambda_k(t) = \lambda_k(t, r)$; they are continuous, monotonically decreasing functions of $t$ and converge to $\mu_k$ 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 agreement with Theorem 1.1. In [HK1] we also discuss muffin tin potentials with dislocation in the $y$ direction.

(2) The rotation problem. In [HK2], we look at three types of muffin tin potentials and discuss the effect of the “filling up” of the gaps at small angles of rotation. We begin with muffin tins with walls of infinite height, then approximate by muffin tin potentials of height $n$, for $n \in \mathbb{N}$ large. By another approximation step, one may obtain examples with Lipschitz-continuous potentials. These examples show, among other things, that Schrödinger operators of the form $R_\theta$ may in fact have spectral gaps for some $\theta > 0$. For the sake of brevity, we only state our main results and refer to [HK2] for further details.

We write (in the notation of (1.5)) $\Omega_r = \Omega_{r, (1/2, 1/2)}$ and

$$\Omega_{r, \theta} := \Omega_r \cap \{x \geq 0\} \cup (M_\theta \Omega_r) \cap \{x < 0\},$$

and let $H_{r, \theta}$ denote the Dirichlet Laplacian on $\Omega_{r, \theta}$, for $0 < r < 1/2$ and $0 \leq \theta \leq \pi/4$. Denote the Dirichlet eigenvalues of the Laplacian $H_r$ of $\Omega_r$ by $(\tilde{\mu}_j(r))_{j \in \mathbb{N}}$, with $\tilde{\mu}_j(r) \to \infty$ as $j \to \infty$ and $\tilde{\mu}_j(r) < \tilde{\mu}_{j+1}(r)$ for all $j \in \mathbb{N}$; note that the eigenvalues $\tilde{\mu}_j$ may have multiplicity $> 1$.

4.1. Proposition. Let $(a, b)$ be one of the gaps $(\tilde{\mu}_j, \tilde{\mu}_{j+1})$ and let $0 < r < 1/2$ be fixed.

(a) Each $\tilde{\mu}_j(r)$, $j = 1, 2, \ldots$, is an eigenvalue of infinite multiplicity of $H_{r, \theta}$, for all $0 \leq \theta \leq \pi/2$. The spectrum of $H_{r, \theta}$ is pure point, for all $0 \leq \theta \leq \pi/2$.

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

(c) There exists a set $\Theta \subset (0, \pi/2)$ of full measure such that $\sigma(H_{r, \theta}) = [\tilde{\mu}_1(r), \infty)$. The eigenvalues different from the $\tilde{\mu}_j(r)$ are of finite multiplicity for $\theta \in \Theta$. 

$R_\theta$ “fills” the gap $(a, b)$ as $0 \neq \theta \to 0$. This implies, in particular, that $R_\theta$ cannot converge to $H$ in the norm resolvent sense, as $\vartheta \to 0$.
4.2. Remark. If $\tan \vartheta$ is rational, the grid $M_\vartheta \mathbb{Z}^2$ is periodic in the $x$- and $y$-directions with $\vartheta$-dependent periods $p, q \in \mathbb{N}$. As a consequence, $H_{r, \vartheta}$ has at most a finite number of eigenvalues in $(a, b)$ for $\vartheta$ rational, each of them of infinite multiplicity. Hence we see a drastic change in the spectrum for $\tan \vartheta \in \mathbb{Q}$ as compared with $\vartheta \in \Theta$. Furthermore, if $\tan \vartheta$ is rational with $\tan \vartheta \notin \{1/(2k+1) \mid k \in \mathbb{N}\}$, then there is some $r_\vartheta > 0$ such that $\sigma(H_{r, \vartheta}) = \sigma(H_r)$ for all $0 < r < r_\vartheta$.

We next turn to muffin tin potentials of finite height. Here we define the potential $V_{r, \vartheta}$ to be zero on $\Omega_{r, \vartheta}$ and $V_{r, \vartheta} = 1$ on the complement of $\Omega_{r, \vartheta}$, where $0 < r < 1/2$ and $0 \leq \vartheta \leq \pi/4$; we also let $H_{r, n, \vartheta} := H_0 + nV_{r, \vartheta}$. The periodic operators $H_{r, n, \vartheta}$ have purely absolutely continuous spectrum and $H_{r, n, \vartheta} \to H_{r, \vartheta}$ in the sense of norm resolvent convergence, uniformly for $\vartheta \in [0, \pi/4]$.

4.3. Proposition. Let $(a, b)$ be one of the gaps $(\mu_j, \mu_{j+1})$. We then have:

(a) For $\tan \vartheta \in \mathbb{Q}$ the spectrum of $H_{r, n, \vartheta}$ has gaps inside the interval $(a, b)$ for $n$ large. More precisely, if $H_{r, \vartheta}$ has a gap $(a', b') \subset (a, b)$, then, for $\varepsilon > 0$ given, the interval $(a' + \varepsilon, b' - \varepsilon)$ will be free of spectrum of $H_{r, n, \vartheta}$ for $n$ large.

(b) For any $\varepsilon > 0$ there are $\vartheta_0 > 0$ and $n_0 > 0$ such that any interval $(c - \varepsilon, c + \varepsilon) \subset (a, b)$ contains spectrum of $H_{r, n, \vartheta}$ for all $0 < \vartheta < \vartheta_0$ and $n \geq n_0$.

By similar arguments, we can approximate $V_{r, \vartheta}$ by Lipschitz-continuous muffin tin potentials that converge monotonically (from below) to $V_{r, \vartheta}$ in such a way that norm resolvent convergence holds for the associated Schrödinger operators (again uniformly in $\vartheta \in [0, \pi/4]$). The spectral properties obtained are analogous to the ones stated in Proposition 4.3. Note, however, that the statement corresponding to part (b) in Proposition 4.3 is weaker than the result of our main Theorem 1.1.

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