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NUMERICAL RECONSTRUCTION OF THE FIRST BAND(S) IN AN INVERSE HILL'S PROBLEM

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Abstract. This paper concerns an inverse band structure problem for one dimensional periodic Schrödinger operators (Hill's operators). Our goal is to find a potential for the Hill's operator in order to reproduce as best as possible some given target bands, which may not be realisable. We recast the problem as an optimisation problem, and prove that this problem is well-posed when considering singular potentials (Borel measures).

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1. Introduction

The aim of this article is to present new considerations on an inverse band structure problem for periodic one-dimensional Schrödinger operators, also called Hill's operators. A Hill operator is a self-adjoint, bounded from below operator of the form $A^V := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$, acting on $L^2(\mathbb{R})$, and where V is a periodic real-valued potential. Its spectrum is composed of a reunion of intervals, which can be characterised using Bloch–Floquet theory as the reunion of the spectra of a family of self-adjoint compact resolvent operators A_q^V, indexed by an element $q \in \mathbb{R}$ called the *quasi-momentum* or *k-point* (see [21], Chap. XIII and Sect. 2.1). For each $q \in \mathbb{R}$, the spectrum of A_q^V is a non-decreasing sequence of eigenvalues $(\varepsilon_{q,n}^V)_{n\in\mathbb{N}^*}$ going to infinity as $n \to +\infty$. For any $m \in \mathbb{N}^*$, the function $\mathbb{R} \ni q \mapsto \varepsilon_{q,m}^V$ is called the mth band function associated to the periodic potential V. The properties of these band functions are well-known, especially in the one-dimensional case (see *e.g.* [21], Chap. XIII).

The optimisation of the band structure of such Hill's operators is an interesting mathematical question of practical interest, which can be roughly formulated as follows: *is it possible to find a potential V so that its M first bands $(\varepsilon_{q,m}^V)_{1\leq m\leq M}$ are close to some target functions $(b_m(q))_{1\leq m\leq M}$?*

A wide mathematical literature answers the question when the target functions are indeed the bands of some Hill's operator, corresponding to some V_{ref} (*i.e.* when $b_m(q) = \varepsilon_{q,m}^{V_{\mathrm{ref}}}$). In this case, we need to *recover* a potential V that reproduces the bands of V_{ref}. This problem is called an *inverse spectral problem*. We refer to [3–5, 7, 20, 23] for the case when V_{ref} is a regular potential, and to [11–15] when V_{ref} is singular (see also the review [17]). The main ideas of the previous references are as follows. First, the band structure of a Hill's

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operator can be seen as the transformation of an analytic function. In particular, the knowledge of any band on an open set is enough to recover *theoretically* the whole band structure. A potential is then reconstructed from the high energy asymptotics of the bands.

The previous methods use the knowledge of the behaviour of the high energy bands, and therefore are unsuitable for practical purpose (material design) since we usually have no accurate and numerically stable information about these high energy bands. Moreover, in practice, only the low energy bands are usually of interest, and are generally computed only on a finite set of quasi-momenta. An additional difficulty is the following: there exists no explicit characterisation of the set of functions $\left\{\varepsilon^V_{q,m}\right\}_{1\leq m\leq M}$ for a reasonable class of potentials V. For applications, it is interesting to know how to construct a potential such that only its first bands are close to some given target functions, which may not be realisable (for instance not analytic). Such an issue arises for instance for the design of photovoltaic materials. Indeed, the efficiency of a crystalline solar cell depends on the band structures of the semiconducting materials entering its composition. The proposed work can be seen as a simplified version of this question. Identifying a periodic potential is a first (yet not sufficient) hint to the identification of an *optimal* material (which should ideally be described by its chemical composition).

In this work, we recast the inverse problem as an optimisation problem. More precisely, for a given set of target functions $(b_m(q))_{1\leq m\leq M}$, we look for a potential V that minimises the error $\sum_{m=1}^M \int_q |b_m(q)-\varepsilon^V_{q,m}|^2\,\mathrm{d}q$. Our main result (Thm. 2.3) states that there exists at least one minimiser, in the case $M=1$, in some class of singular potentials. Of course, this minimiser cannot be unique, due to the well-known isospectrality properties of one-dimensional Schrödinger operators (see for instance [21], Thm. XIII.93). The second part of this work is devoted to the numerical resolution of this minimisation problem. Two main issues arise when it comes to practice: handling non-uniqueness of minimising potentials, and the fact that they might be singular. A natural choice (which we make) consists in discretising periodic potentials in Fourier series. In this work, we investigate how the choice of the Fourier cut-off affects the approximation of the bands. To the best of our knowledge, this is the first time that such a least-square problem is considered from a theoretical or numerical point of view. Let us mention here that other approaches, based on genetic algorithms, have been considered in the physics and chemistry literature [24]. The latter are mainly data-driven and require the use of a large amount of true experimental measures.

The outline of the paper is as follows. In Section 2, we recall basic properties about Hill's operators with singular potentials and we state our main result (Thm. 2.3). Its proof is given in Section 3. Finally, we present in Section 4 some numerical tests which illustrate some of our theoretical results.

2. Spectral decomposition of periodic Schrödinger operators, and main results

In this section, we recall some properties of Hill's operators with singular potentials. Elementary notions on the Bloch-Floquet transform [21] are gathered in Section 2.1. The spectral decomposition of one-dimensional periodic Schrödinger operators with singular potentials is detailed in Section 2.2, building on the results of [2, 9, 10, 16, 19]. We state our main results in Section 2.3.

2.1. Bloch-Floquet transform

We need some notation. Let $\mathcal{D}'$ denotes the Schwartz space of complex-valued distributions, and let $\mathcal{D}'_{\mathrm{per}}\subset\mathcal{D}'$ be the space of distributions that are 2π-periodic. In the sequel, the unit cell is $\Gamma:=[-\pi,\pi)$, and the reciprocal unit cell (or Brillouin zone) is $\Gamma^*:=[-1/2,1/2]$. For $u\in\mathcal{D}'_{\mathrm{per}}$ and $k\in\mathbb{Z}$, the kth normalised Fourier coefficient of u is denoted by $\widehat{u}(k)$. For $s\in\mathbb{R}$, we denote by

$$H^s_{\mathrm{per}}:=\left\{u\in\mathcal{D}'_{\mathrm{per}},\ \|u\|^2_{H^s_{\mathrm{per}}}:=\sum_{k\in\mathbb{Z}}(1+|k|^2)^s|\widehat{u}(k)|^2<+\infty\right\}$$

the complex-valued periodic Sobolev space, which is a Hilbert space when endowed with its natural inner product. We write $H^s_{\mathrm{per},r}$ for the *real-valued* periodic Sobolev space, *i.e.*

$$H^s_{\mathrm{per},r} := \left\{ u \in H^s_{\mathrm{per}}, \quad \forall k \in \mathbb{Z},\ \widehat{u}(-k) = \overline{\widehat{u}(k)} \right\}.$$

We also let $L^2_{\mathrm{per}} := H^{s=0}_{\mathrm{per}}$. From our normalisation, it holds that

$$\forall v, w \in L^2_{\mathrm{per}},\ \langle v, w \rangle_{L^2_{\mathrm{per}}} = \int_\Gamma \overline{v} w \quad \text{and} \quad \forall v, w \in H^1_{\mathrm{per}},\ \langle v, w \rangle_{H^1_{\mathrm{per}}} = \int_\Gamma \frac{\mathrm{d}\overline{v}}{\mathrm{d}x} \frac{\mathrm{d}w}{\mathrm{d}x} + \int_\Gamma \overline{v} w.$$

Lastly, we denote by C^0_{per} the space of 2π-periodic continuous functions, and by C^∞_c the space of C^∞ functions over $\mathbb{R}$, with compact support.

To introduce the Bloch-Floquet transform, we let $\mathcal{H} := L^2(\Gamma^*, L^2_{\mathrm{per}})$. For any element $f \in \mathcal{H}$, we denote by $f_q(x)$ its value at the point $(q, x) \in \Gamma^* \times \Gamma$. The space $\mathcal{H}$ is an Hilbert space when endowed with its inner product

$$\forall f, g \in \mathcal{H}, \quad \langle f, g \rangle_{\mathcal{H}} := \int_{\Gamma^*} \int_\Gamma \overline{f_q(x)} g_q(x) \mathrm{d}x\ \mathrm{d}q.$$

The Bloch-Floquet transform is the map $\mathcal{B} : L^2(\mathbb{R}) \to \mathcal{H}$ defined, for smooth functions $\varphi \in C^\infty_c(\mathbb{R})$, by

$$\phi_q(x) := (\mathcal{B}\varphi)_q(x) := \sum_{R \in \mathbb{Z}} \varphi(x + R) e^{-\mathrm{i}q(R+x)}.$$

It is an isometry from $L^2(\mathbb{R})$ to $\mathcal{H}$, whose inverse is given by

$$\left(\mathcal{B}^{-1}\phi\right)(x) := \int_{\Gamma^*} \phi_q(x) e^{iqx}\, \mathrm{d}q = \varphi(x).$$

The Bloch theorem states that if A is a self-adjoint operator on $L^2(\mathbb{R})$ with domain $D(A)$ that commutes with $\mathbb{Z}$-translations, then $\mathcal{B}A\mathcal{B}^{-1}$ is diagonal in the q-variable. More precisely, there exists a unique family of self-adjoint operators $(A_q)_{q \in \Gamma^*}$ on L^2_{per} such that for all $\varphi \in L^2(\mathbb{R}) \cap D(A)$,

$$(A\varphi)(x) = \int_{\Gamma^*} (A_q \phi_q)(x)\, \mathrm{d}q.$$

In this case, we write

$$A = \int_{\Gamma^*}^{\oplus} A_q \mathrm{d}q.$$

2.2. Hill's operators with singular potentials

Giving a rigorous mathematical sense to a Hill's operator of the form $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ on $L^2(\mathbb{R})$, when the potential V is singular is not an obvious task. In the present paper, we consider $V \in H^{-1}_{\mathrm{per,r}}$, which is a case that was first tackled in [16] (see also [2, 9, 10, 19] for recent results).

The results which are gathered in this section are direct corollaries of results which were proved in these earlier works, particularly in [10].

Proposition 2.1. [[10], Thm. 2.1 and Lem. 3.2] *For all $V \in H^{-1}_{\mathrm{per,r}}$, there exists $\sigma_V \in L^2_{\mathrm{per}}$ and $\kappa_V \in \mathbb{R}$ such that*

$$V = \sigma_V' + \kappa_V \text{ in } \mathcal{D}'_{\mathrm{per}}. \tag{2.1}$$

Moreover, if $a^V : H^1(\mathbb{R}) \times H^1(\mathbb{R}) \to \mathbb{C}$ is the sesquilinear form defined by

$$\forall v, w \in H^1(\mathbb{R}), \quad a^V(v,w) = \int_{\mathbb{R}} \frac{\mathrm{d}\overline{v}}{\mathrm{d}x}\,\frac{\mathrm{d}w}{\mathrm{d}x} + \int_{\mathbb{R}} \kappa_V \overline{v} w - \int_{\mathbb{R}} \sigma_V \left(\frac{\mathrm{d}\overline{v}}{\mathrm{d}x} w + \overline{v}\frac{\mathrm{d}w}{\mathrm{d}x}\right), \tag{2.2}$$

then a^V is a symmetric, continuous sesquilinear form on $H^1(\mathbb{R}) \times H^1(\mathbb{R})$, which is closed and bounded from below. Besides, a^V is independent of the choice of $\sigma_V \in L^2_{\mathrm{per}}$ and $\kappa_V \in \mathbb{R}$ satisfying (2.1).

Remark 2.2. The expression (2.2) makes sense whenever $v, w \in H^1(\mathbb{R})$. This can be easily seen with the Cauchy-Schwarz inequality, and the embedding $H^1(\mathbb{R}) \hookrightarrow L^\infty(\mathbb{R})$. It is not obvious how to extend this result to higher dimension.

A direct consequence of Proposition 2.1 is that one can consider the Friedrichs operator on $L^2(\mathbb{R})$ associated to a^V, which is denoted by A^V in the sequel. The operator A^V is thus a densely defined, self-adjoint, bounded from below operator on $L^2(\mathbb{R})$, with form domain $H^1(\mathbb{R})$ and whose domain is dense in $L^2(\mathbb{R})$. Formally, it holds that

$$A^V = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V.$$

The spectral properties of the operator A^V can be studied (like in the case of regular potentials) using Bloch-Floquet theory.

The previous result, together with Bloch-Floquet theory, allows to study the operator A^V *via* its Bloch fibers $\left(A^V_q\right)_{q\in\Gamma^*}$. For $q \in \Gamma^*$, it holds that A^V_q is the self-adjoint extension of the operator

$$\left|-i\frac{\mathrm{d}}{\mathrm{d}x} + q\right|^2 + V.$$

It holds that A^V_q is a bounded from below self-adjoint operator acting on L^2_{per}, whose form domain is H^1_{per}, and with associated quadratic form a^V_q, defined by (recall that H^1_{per} is an algebra)

$$\forall v, w \in H^1_{\mathrm{per}}, \quad a^V_q(v,w) := \int_\Gamma \left[\overline{\left(-i\frac{\mathrm{d}}{\mathrm{d}x} + q\right) v}\left(-i\frac{\mathrm{d}}{\mathrm{d}x} + q\right) w\right] + \langle V, \overline{v} w\rangle_{H^{-1}_{\mathrm{per}}, H^1_{\mathrm{per}}}. \tag{2.3}$$

In other words, we have

$$A^V = \int_{\Gamma^*}^{\oplus} A^V_q \,\mathrm{d}q.$$

The fact that L^2_{per} is compactly embedded in H^1_{per} implies that A^V_q is compact-resolvent. As a consequence, there exists a non-decreasing sequence of real eigenvalues $\left(\varepsilon^V_{q,m}\right)_{m\in\mathbb{N}^*}$ going to $+\infty$ and a corresponding orthonormal basis $(u^V_{q,m})_{m\in\mathbb{N}^*}$ of L^2_{per} such that

$$\forall m \in \mathbb{N}^*, \quad A^V_q u^V_{q,m} = \varepsilon^V_{q,m} u^V_{q,m}. \tag{2.4}$$

The map $\Gamma^* \ni q \mapsto \varepsilon_{q,m}^V$ is called the mth band. Since the potential V is real-valued, it holds that $A_{-q}^V = \overline{A_q^V}$, so that $\varepsilon_{-q,m}^V = \varepsilon_{q,m}^V$ for all $q \in \Gamma^*$ and $m \in \mathbb{N}^*$. This implies that it is enough to study the bands on $[0, 1/2]$. Actually, we have

$$\sigma(A^V) = \bigcup_{q\in[0,1/2]} \bigcup_{m\in\mathbb{N}^*} \{\varepsilon_{q,m}^V\}.$$

In the sequel, we mainly focus on the first band. We write $\varepsilon_q^V := \varepsilon_{q,1}^V$ for the sake of clarity. Thanks to the knowledge of the form domain of A_q^V, we know that

$$\varepsilon_q^V := \min_{\substack{v\in H^1_{\mathrm{per}} \\ \|v\|_{L^2_{\mathrm{per}}}=1}} a_q^V(v,v). \tag{2.5}$$

This characterisation will be the key to our proof. When the potential V is smooth (say $V \in L^2_{\mathrm{per}}$), then the map $\Gamma^* \ni q \mapsto \varepsilon_{q,m}^V$ is analytic on $(-1/2, 1/2)$. Besides, it is increasing on $[0, 1/2]$ if m is odd, and decreasing if m is even (see *e.g.* [21], Chap. XIII).

2.3. Main results

The goal of this article is to find a potential V so that the bands of the corresponding Hill's operator are close to some given target functions. In order to do so, we recast the problem as a minimisation one, of the form

$$V^* \in \arg\min_{V\in\mathcal{V}} \mathcal{J}(V).$$

Unfortunately, we were not able to consider the full setting where the minimisation set $\mathcal{V}$ is the whole set $H^{-1}_{\mathrm{per},r}$. The problem was that we were unable to control the negative part of V. To bypass this difficulty, we chose to work with potentials that are bounded from below. Such a distribution is necessary a measure (see *e.g.* [18]). Hence measure-valued potentials provide a natural setting for band reconstruction. We recall here some basic properties about measures.

We denote by $\mathcal{M}^+_{\mathrm{per}}$ the space of non-negative 2π-periodic regular Borel measures on $\mathbb{R}$, in the sense that for all $\nu \in \mathcal{M}^+_{\mathrm{per}}$, and all Borel set $S \in \mathcal{B}(\mathbb{R})$, it holds that $\nu(S) = \nu(S + 2\pi) \geq 0$, and $\nu(\Gamma) < \infty$. For all $\epsilon > 0$, from the Sobolev embedding $H^{1/2+\varepsilon}_{\mathrm{per}} \hookrightarrow C^0_{\mathrm{per}}$, we deduce that $\mathcal{M}^+_{\mathrm{per}} \hookrightarrow H^{-1/2-\varepsilon}_{\mathrm{per}} \hookrightarrow H^{-1}_{\mathrm{per}}$, where the last embedding is compact. For $\nu \in \mathcal{M}^+_{\mathrm{per}}$, we denote by $V_\nu \in H^{-1}_{\mathrm{per},r}$ the unique corresponding potential, which is defined by duality through the relation:

$$\forall \phi \in H^1_{\mathrm{per}}, \quad \int_\Gamma \phi \mathrm{d}\nu = \langle V_\nu, \phi\rangle_{H^{-1}_{\mathrm{per}}, H^1_{\mathrm{per}}}.$$

For $B \in \mathbb{R}$, we define the set of B-bounded from below potentials

$$\mathcal{V}_B := \left\{V \in H^{-1}_{\mathrm{per},r} | \quad \exists \nu \in \mathcal{M}^+_{\mathrm{per}}, \quad V = V_\nu - B\right\} \subset H^{-1}_{\mathrm{per,r}}.$$

This will be our minimisation space for our optimisation problem. Note that $\mathcal{V}_{B_1} \subset \mathcal{V}_{B_2}$ for $B_1 \geq B_2$.

We now introduce the functional $\mathcal{J}$ to minimise. First, we introduce the set $\mathcal{T}$ of allowed target functions:

$$\mathcal{T} := \left\{b \in C^0(\Gamma^*), \quad b \text{ is even and } b \text{ is increasing on } [0, 1/2]\right\}. \tag{2.6}$$

Of course, for all $V \in H^{-1}_{\mathrm{per},r}$, it holds that $\Gamma^* \ni q \mapsto \varepsilon_q^V \in \mathcal{T}$. Finally, in order to quantify the quality of reconstruction of a band $b \in \mathcal{T}$, we introduce the error functional $\mathcal{J}_b : H^{-1}_{\mathrm{per,r}} \to \mathbb{R}$ defined by

$$\forall V \in H^{-1}_{\mathrm{per,r}}, \quad \mathcal{J}_b(V) := \frac{1}{2}\int_{\Gamma^*} |b(q) - \varepsilon_q^V|^2 \,\mathrm{d}q = \int_0^{1/2} |b(q) - \varepsilon_q^V|^2 \,\mathrm{d}q. \tag{2.7}$$

The main result of the present paper is the following.

Theorem 2.3. *Let $b \in \mathcal{T}$, and denote by $b^* := \fint_{\Gamma^*} b(q)\,\mathrm{d}q \in \mathbb{R}$. Then, for all $B > 1/4 - b^*$, there exists a solution $V_{b,B} \in \mathcal{V}_B$ to the minimisation problem*

$$V_{b,B} \in \operatorname*{arg\,min}_{V \in \mathcal{V}_B} \mathcal{J}_b(V). \tag{2.8}$$

Remark 2.4. Uniqueness cannot be expected due to the isospectrality properties of one-dimensional periodic Schrödinger operators ([21], Chap. XIII). For instance, the potentials $V(\cdot + \tau)$ and $V(\cdot)$ have the same band structure for any $\tau \in \mathbb{R}$. In addition, for all $t \geq 0$, the potential $V(t, \cdot)$ also has the same band structure, where $V(t, x)$ is the solution of the Korteweg-de Vries equation [8]

$$\partial_t V = 3V\partial_x V - \frac{1}{2}\partial_{xxx} V, \quad V(t = 0, \cdot) = V_0.$$

The proof of Theorem 2.3 relies on the following proposition, which is central to our analysis. Both the proofs of Theorem 2.3 and Proposition 2.5 are provided in the next section.

Proposition 2.5. *Let $B \in \mathbb{R}$ and let $(V_n)_{n\in\mathbb{N}^*} \subset \mathcal{V}_B$. For all $n \in \mathbb{N}^*$, let $\nu_n \in \mathcal{M}^+_{\mathrm{per}}$ such that $V_n := V_{\nu_n} - B$. Let us assume that the sequence $\left(\varepsilon_0^{V_n}\right)_{n\in\mathbb{N}^*}$ is bounded and such that $\nu_n(\Gamma) \underset{n\to+\infty}{\longrightarrow} +\infty$. Then, up to a subsequence (still denoted n), the functions $q \mapsto \varepsilon_q^{V_n}$ converge uniformly to a constant function $\varepsilon \in \mathbb{R}$, with $\varepsilon \geq \frac{1}{4} - B$. In other words, there is $\varepsilon \geq \frac{1}{4} - B$ such that*

$$\max_{q\in[0,1/2]} \left|\varepsilon_q^{V_n} - \varepsilon\right| \underset{n\to\infty}{\longrightarrow} 0. \tag{2.9}$$

Conversely, for all $\varepsilon \geq \frac{1}{4} - B$, there is a sequence $(V_n)_{n\in\mathbb{N}^*} \subset \mathcal{V}_B$ such that (2.9) holds.

This result implies that the first band of the sequence of operators $\left(A^{V_n}\right)_{n\in\mathbb{N}^*}$, where $(V_n)_{n\in\mathbb{N}^*}$ satisfies the assumptions of Proposition 2.5, *becomes flat.*

Remark 2.6. Here we have a sequence of first bands $\left(\varepsilon_q^{V_n}\right)_{n\in\mathbb{N}^*}$ that converges uniformly to a constant function. However, as the first band of any Hill's operator must be increasing and analytic, the limit *is not* the first band of a Hill's operator.

3. Proof of Theorem 2.3 and Proposition 2.5

3.1. Preliminary lemmas

We first prove some intermediate useful lemmas before giving the proof of Proposition 2.5 and Theorem 2.3. We start by recording a spectral convergence result.

Proposition 3.1. [[10], Thm. 4.1] *Let $(V_n)_{n\in\mathbb{N}^*} \subset H^{-1}_{\mathrm{per},r}$ be a sequence such that $(V_n)_{n\in\mathbb{N}^*}$ converges strongly in H^{-1}_{per} to some $V \in H^{-1}_{\mathrm{per},r}$. Then,*

$$\forall m \in \mathbb{N}^*, \quad \max_{q\in[0,1/2]} \left|\varepsilon_{q,m}^{V_n} - \varepsilon_{q,m}^{V}\right| \underset{n\to\infty}{\longrightarrow} 0.$$

In our case, since we are working with potentials that are measures, we deduce the following result.

Proposition 3.2. *Let $B \in \mathbb{R}$ and $(V_n)_{n\in\mathbb{N}^*} \subset \mathcal{V}_B$ be a bounded sequence, in the sense*

$$\sup_{n\in\mathbb{N}} \langle V_n, \mathbb{1}_\Gamma\rangle_{H^{-1}_{\mathrm{per}},H^1_{\mathrm{per}}} < \infty.$$

For all $n \in \mathbb{N}^*$, let $\nu_n \in \mathcal{M}^+_{\mathrm{per}}$ such that $V_n = V_{\nu_n} - B$. Then, there exists $\nu \in \mathcal{M}^+_{\mathrm{per}}$ such that, up to a subsequence (still denoted n), $(\nu_n)_{n\in\mathbb{N}}$ converges weakly- to ν in $\mathcal{M}_{\mathrm{per}}$, and $(V_n)_{n\in\mathbb{N}^*}$ converges strongly in H^{-1}_{per} to $V := V_\nu - B \in \mathcal{V}_B$. Moreover, we have*

$$\forall m \in \mathbb{N}^*, \quad \max_{q\in[0,1/2]} \left|\varepsilon^{V_n}_{q,m} - \varepsilon^{V}_{q,m}\right| \xrightarrow[n\to\infty]{} 0.$$

Proof. The fact that we can extract from the bounded sequence $(\nu_n)_{n\in\mathbb{N}^*}$ a weakly-* convergent sequence in $\mathcal{M}^+_{\mathrm{per}}$ is the Prokhorov's theorem applied in the torus Γ^*. The second part comes from the compact embedding $\mathcal{M}_{\mathrm{per}} \hookrightarrow H^{-1}_{\mathrm{per}}$. The final part is the direct application of Proposition 3.1. □

Remark 3.3. This proposition explains our choice to consider measure-valued potentials. Note that a similar result does not hold in the L^1_{per} setting for instance.

We now give a lemma which is standard in the case of regular potentials V (see [6]).

Lemma 3.4. *Let $V \in \mathcal{V}_B$ for some $B \in \mathbb{R}$. The first eigenvector $u^V_{q=0} \in H^1_{\mathrm{per}}$ of $A^V_{q=0}$ is unique up to a global phase. It can be chosen real-valued and positive.*

Proof. We use the min-max principle (2.5), and the fact that, for $u \in H^1_{\mathrm{per}}$, the following holds

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}|u|\right| \leq \left|\frac{\mathrm{d}}{\mathrm{d}x}u\right| \quad \text{a.e.}$$

We see that if u is an eigenvector corresponding to the first eigenvalue, then so is $|u|$. We now consider a non-negative eigenvector $u \geq 0$, and prove that it is positive. The usual argument is Harnack's inequality. However, it is *a priori* unclear that it works in our singular setting. To prove it, we write $V = V_\nu - B$ for $\nu \in \mathcal{M}^+_{\mathrm{per}}$, and consider the repartition function F_ν of ν: $F_\nu(x) := \nu((0,x])$. This function is not periodic, but the function $f_\nu(x) := F_\nu(x) - \nu(\Gamma)\frac{x}{|\Gamma|}$ is. Since F_ν is an non decreasing, right-continuous function, we deduce that $f_\nu \in L^\infty_{\mathrm{per}}$. Moreover, it holds, in the H^{-1}_{per} sense, that $f'_\nu = V_\nu - |\Gamma|^{-1}\nu(\Gamma) = V + B - |\Gamma|^{-1}\nu(\Gamma)$. As a result, we see that u is solution to the minimisation problem

$$u \in \operatorname*{arg\,min}_{\substack{v\in H^1_{\mathrm{per},r}\\ \|v\|_{L^2_{\mathrm{per}}}=1}} \left\{ \int_\Gamma \left|\frac{\mathrm{d}v}{\mathrm{d}x}\right|^2 + \left(\frac{\nu(\Gamma)}{|\Gamma|} - B\right) - 2\int_\Gamma f_\nu \left(v\frac{\mathrm{d}v}{\mathrm{d}x}\right)\right\}.$$

There exists $\lambda \in \mathbb{R}$ so that the corresponding Euler-Lagrange equations can be written in the weak-form:

$$\operatorname{div} F(x,u,u') + G(x,u,u') = 0,$$

with

$$F(x,u,p) = p - f_\nu u \quad \text{and} \quad G(x,u,p) = f_\nu p + \lambda u.$$

We are now in the settings of ([22], Thm. 1.1), and we deduce that $u > 0$. The rest of the proof is standard. □

3.2. Proof of Proposition 2.5

We now prove Proposition 2.5. Let $B \in \mathbb{R}$ and let $V_n = V_{\nu_n} - B \in \mathcal{V}_B$ with $\nu_n \in \mathcal{M}^+_{\mathrm{per}}$, be a sequence such that the sequence $\left(\varepsilon^{V_n}_{q=0}\right)_{n\in\mathbb{N}^*}$ is bounded and $\nu_n(\Gamma)$ goes to $+\infty$. Since $\left(\varepsilon^{V_n}_0\right)_{n\in\mathbb{N}^*}$ is bounded, then up to a subsequence (still denoted by n), there exists $\varepsilon \in \mathbb{R}$ such that $\varepsilon^{V_n}_0$ converges to ε. Our goal is to prove that the convergence also holds uniformly in $q \in \Gamma^*$.

Let $u^{V_n}_0 \in H^1_{\mathrm{per}}$ be the L^2_{per}-normalised positive eigenvector of $A^{V_n}_0$ associated to the eigenvalue $\varepsilon^{V_n}_0$ (see Lem. 3.4). We denote by $\alpha_n := \min_{x\in\Gamma} u^{V_n}_0(x) > 0$. Let us first prove that the following convergences hold:

$$\alpha_n \int_\Gamma u^{V_n}_0 \,\mathrm{d}\nu_n \xrightarrow[n\to+\infty]{} 0 \quad \text{and} \quad \alpha_n^2 \nu_n(\Gamma) \xrightarrow[n\to+\infty]{} 0. \tag{3.1}$$

From the equality

$$\int_\Gamma \left|\frac{\mathrm{d}}{\mathrm{d}x}\left(u^{V_n}_0\right)\right|^2 + \int_\Gamma |u^{V_n}_0|^2 \mathrm{d}\nu_n = \varepsilon^{V_n}_0 + B,$$

we get

$$\alpha_n^2 \nu_n(\Gamma) \le \alpha_n \int_\Gamma u^{V_n}_0 \mathrm{d}\nu_n \le \int_\Gamma |u^{V_n}_0|^2 \mathrm{d}\nu_n \le \varepsilon^{V_n}_0 + B. \tag{3.2}$$

As the right-hand side is bounded, and $\nu_n(\Gamma) \to +\infty$ by hypothesis, this implies $\alpha_n \to 0$. Moreover, we have

$$0 \le \int_\Gamma u^{V_n}_0 \,\mathrm{d}\nu_n = a^{V_n}_0(u^{V_n}_0, \mathbb{1}_\Gamma) + B\int_\Gamma u^{V_n}_0 = (\varepsilon^{V_n}_0 + B)\int_\Gamma u^{V_n}_0 \le (\varepsilon^{V_n}_0 + B)|\Gamma|^{1/2},$$

where we used the Cauchy-Schwarz inequality for the last part. As a result, we deduce that the sequence $\left(\int_\Gamma u^{V_n}_0 \,\mathrm{d}\nu_n\right)_{n\in\mathbb{N}^*}$ is bounded. The first convergence of (3.1) follows. The second convergence is a consequence of the first inequality in (3.2).

Let $x_n \in \Gamma = [0, 2\pi)$ be such that $\alpha_n = u^{V_n}_0(x_n)$. The fact that $\alpha_n \to 0$ implies that $l_n := \|u^{V_n}_0(x_n + \cdot) - \alpha_n\|^2_{L^2_{\mathrm{per}}} \to 1$ and we can thus define for n large enough

$$v_n := \frac{u^{V_n}_0(x_n + \cdot) - \alpha_n}{\|u^{V_n}_0(x_n + \cdot) - \alpha_n\|_{L^2_{\mathrm{per}}}}.$$

It holds that $v_n \in H^1_{\mathrm{per}}$, $\|v_n\|_{L^2_{\mathrm{per}}} = 1$. Besides, we have $v_n(0) = 0$. For $q \in \Gamma^*$, we introduce the function $v_{q,n}$ defined by:

$$\forall x \in \mathbb{R}, \quad v_{q,n}(x) := v_n(x)e^{-iq[x]}, \quad \text{where we set} \quad [x] := x \bmod 2\pi.$$

Thanks to the equality $v_n(0) = 0$, it holds that $v_{q,n} \in H^1_{\mathrm{per}}$, and that $\|v_{q,n}\|_{L^2_{\mathrm{per}}} = 1$. This function is therefore a valid test function for our min–max principle.[1]

[1] This construction only works in one dimension. We do not know how to construct similar test functions in higher dimension.

From the min–max principle (2.5) and the expression (2.3), we obtain

$$\begin{aligned}
B+\varepsilon_q^{V_n} &\le B + a_q^{V_n}(v_{q,n},v_{q,n}) \\
&= \int_\Gamma \left|\left(-i\frac{\mathrm{d}}{\mathrm{d}x}+q\right)v_{q,n}\right|^2 + \int_\Gamma |v_{q,n}|^2\,\mathrm{d}\nu_n = \int_\Gamma \left|\frac{\mathrm{d}v_n}{\mathrm{d}x}\right|^2 + \int_\Gamma |v_n|^2\,\mathrm{d}\nu_n \\
&= \frac{1}{l_n}\left(\int_\Gamma \left|\frac{\mathrm{d}}{\mathrm{d}x}\left(u_0^{V_n}(x_n+\cdot)\right)\right|^2 + \int_\Gamma |u_0^{V_n}(x_n+\cdot)-\alpha_n|^2\,\mathrm{d}\nu_n\right) \\
&= \frac{1}{l_n}\left(\int_\Gamma \left|\frac{\mathrm{d}}{\mathrm{d}x}\left(u_0^{V_n}\right)\right|^2 + \int_\Gamma |u_0^{V_n}|^2\,\mathrm{d}\nu_n - 2\alpha_n\int_\Gamma u_0^{V_n}\,\mathrm{d}\nu_n + \alpha_n^2\nu_n(\Gamma)\right) \\
&= \frac{1}{l_n}\left(B+\varepsilon_0^{V_n} - 2\alpha_n\int_\Gamma u_0^{V_n}\,\mathrm{d}\nu_n + \alpha_n^2\nu_n(\Gamma)\right).
\end{aligned}$$

We infer from these inequalities, and from (3.1) that

$$0 \le \max_{q\in\Gamma^*}\left|\varepsilon_q^{V_n}-\varepsilon_0^{V_n}\right| \le \left(B+\varepsilon_0^{V_n}\right)\left(\frac{1}{l_n}-1\right) + \frac{1}{l_n}\left(-2\alpha_n\int_\Gamma u_0^{V_n}\,\mathrm{d}\nu_n + \alpha_n^2\nu_n(\Gamma)\right) \xrightarrow[n\to+\infty]{} 0.$$

This already proves the convergence (2.9).

To see that $\varepsilon \ge \frac{1}{4} - B$, we write, for $V = V_\nu - B$ with $\nu \in \mathcal{M}^+_{\mathrm{per}}$ that

$$\forall q \in [-1/2,1/2], \quad A_q^V = \left|-i\frac{\mathrm{d}}{\mathrm{d}x}+q\right|^2 + V_\nu - B \ge \left|-i\frac{\mathrm{d}}{\mathrm{d}x}+q\right|^2 - B \ge q^2 - B,$$

where we used the fact that the lowest eigenvalue of $\left|-i\frac{\mathrm{d}}{\mathrm{d}x}+q\right|^2$ is q^2 for $q \in [-1/2,1/2]$ (this can be seen with the Fourier representation of the operator). As a consequence, for $q=\frac{1}{2}$, we obtain that for all $V \in \mathcal{V}_B$, $\varepsilon^V_{q=1/2} \ge \frac{1}{4} - B$. The result follows.

To prove the converse, we exhibit an explicit sequence of measures $(\nu_n)_{n\in\mathbb{N}^*} \subset \mathcal{M}^+_{\mathrm{per}}$ such that $\varepsilon_q^{V_{\nu_n}} \to \frac{1}{4}$. The general result will follow by taking sequences of the form $V_n = V_{\nu_n} + \left(\varepsilon - \frac{1}{4}\right) - B$. We denote by δ_x the Dirac mass at $x \in \mathbb{R}$, and consider, for $\lambda > 0$, the measure

$$\nu_\lambda := \lambda \sum_{k\in\mathbb{Z}} \delta_{2\pi k} \in \mathcal{M}^+_{\mathrm{per}}. \tag{3.3}$$

From the first part of the Proposition, it is enough to check the convergence for $q = 0$. We are looking for a solution to (we denote by $\omega_\lambda^2 := \varepsilon_0^{V_{\nu_\lambda}} \ge 0$ for simplicity)

$$-u'' + \lambda\delta_0 u(0) = \omega_\lambda^2 u, \quad u \ge 0, \quad u(2\pi) = u(0). \tag{3.4}$$

On $(0,2\pi)$, u satisfies the elliptic equation $-u'' = \omega_\lambda^2 u$, hence is of the form

$$u(x) = Ce^{i\omega_\lambda x} + De^{-i\omega_\lambda x},$$

for some $C, D \in \mathbb{R}$. The continuity of u at 2π implies $Ce^{2i\pi\omega_\lambda} + De^{-2i\pi\omega_\lambda} = C + D$. Moreover, integrating (3.4) between 0^- and 0^+ leads to the jump of the derivative $-u'(0) + u'(2\pi) + \lambda u(0) = 0$, or

$$i\omega_\lambda (D - C) + i\omega_\lambda \left(Ce^{2i\pi\omega_\lambda} - De^{-2i\pi\omega_\lambda}\right) + \lambda(C + D) = 0.$$

We deduce that (C, D) is solution to the 2×2 matrix equation

$$\begin{pmatrix} 1 - e^{2i\pi\omega_\lambda} & 1 - e^{-2i\pi\omega_\lambda} \\ -i\omega_\lambda \left(1 - e^{2i\pi\omega_\lambda}\right) + \lambda & i\omega_\lambda \left(1 - e^{-2i\pi\omega_\lambda}\right) + \lambda \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The determinant of the matrix must therefore vanish, which leads to

$$1 = \cos(2\pi\omega_\lambda) + \frac{\lambda}{2} \frac{\sin(2\pi\omega_\lambda)}{\omega_\lambda}. \tag{3.5}$$

As $\lambda \to \infty$, one must have $\omega_\lambda \to 1/2$, or equivalently $\varepsilon_0^{V_{\nu_\lambda}} \to 1/4$. The result follows.

3.3. Proof of Theorem 2.3

We are now in position to give the proof of Theorem 2.3. Let $b \in \mathcal{T}$ and $B > 1/4 - b^*$ where $b^* := \fint_{\Gamma^*} b(q)\,\mathrm{d}q$. Let $V_n = V_{\nu_n} - B \subset \mathcal{V}_B$ be a minimising sequence associated to problem (2.8).

Let us first assume by contradiction that $\nu_n(\Gamma) \to \infty$. Then, according to Proposition 2.5, up to a subsequence (still denoted by n), there exists $\varepsilon \geq \frac{1}{4} - B$ such that $\varepsilon_q^{V_n}$ converges uniformly in $q \in \Gamma^*$ to the constant function ε. Also, from the second part of Proposition 2.5, the fact that $B > \frac{1}{4} - b^*$ and the fact that b^* is the unique minimiser to

$$\inf_{c \in \mathbb{R}} \mathcal{K}_b(c), \tag{3.6}$$

where $\mathcal{K}_b(c) := \int_{[0,1/2]} |b(q) - c|^2\,\mathrm{d}q$ for all $c \in \mathbb{R}$, it must hold that $\varepsilon = b^*$.

We now prove that

$$\inf_{V \in \mathcal{V}_B} \mathcal{J}_b(V) \neq \inf_{c \in \mathbb{R}} \mathcal{K}_b(c) = \mathcal{K}_b(b^*).$$

To this aim, we exhibit a potential $W \in \mathcal{V}_B$ such that $\mathcal{J}_b(W) < \mathcal{K}_b(b^*)$. Since b is continuous and increasing on $[0, 1/2]$, there exists a unique $q^* \in (0, 1/2)$ such that $b(q^*) = b^*$. We choose $\delta > 0$ small enough such that $0 < q^* - \delta < q^* + \delta < 1/2$, and set

$$\eta^{\mathrm{ext}} := \int_0^{q^*-\delta} |b(q) - b^*|^2\,\mathrm{d}q + \int_{q^*+\delta}^{1/2} |b(q) - b^*|^2\,\mathrm{d}q \quad \text{and} \quad \eta^{\mathrm{int}} := \int_{q^*-\delta}^{q^*+\delta} |b(q) - b^*|^2\,\mathrm{d}q,$$

so that $\mathcal{K}_b(b^*) = \eta^{\mathrm{ext}} + \eta^{\mathrm{int}}$. Since b is increasing and continuous, we have $\eta^{\mathrm{int}} > 0$ and $\eta^{\mathrm{ext}} > 0$, and $b(q^* - \delta) < b^* < b(q^* + \delta)$.

We now choose a constant $\sigma > 0$ such that

$$0 < \sigma < \min\left\{ \frac{\eta^{\mathrm{int}}}{8\delta}, B + b^* - \frac{1}{4}, b^* - b(q^* - \delta), b(q^* + \delta) - b^* \right\}.$$

Let ν_n be the measure defined in (3.3) for $\lambda = n \in \mathbb{N}$, and let

$$\widetilde{W}_n := V_{\nu_n} + b^* - \frac{1}{4}.$$

Since $\varepsilon_q^{\widetilde{W}_n}$ converges to b^* uniformly in Γ^*, there exists $n_0 \in \mathbb{N}^*$ large enough such that

$$\forall q \in \Gamma^*, \quad \left|\varepsilon_q^{\widetilde{W}_{n_0}} - b^*\right| < \sigma/2.$$

We then define

$$W := \widetilde{W}_{n_0} + b^* - \varepsilon_{q^*}^{\widetilde{W}_{n_0}} = V_{\nu_n} + \left[\left(B + b^* - \frac{1}{4}\right) - \left(\varepsilon_{q^*}^{\widetilde{W}_{n_0}} - b^*\right)\right] - B.$$

Since $\sigma < B + b^* - 1/4$, it holds that $W \in \mathcal{V}_B$. Moreover, $b^* - \sigma < \varepsilon_q^W < b^* + \sigma$ for all $q \in \Gamma^*$. Finally, for $q = q^*$, we have $\varepsilon_{q^*}^W = b^*$.

Let us evaluate $\mathcal{J}_b(W)$. We get

$$\mathcal{J}_b(W) = \int_0^{q^*-\delta} |b(q) - \varepsilon_q^W|^2 \, \mathrm{d}q + \int_{q^*-\delta}^{q^*+\delta} |b(q) - \varepsilon_q^W|^2 \, \mathrm{d}q + \int_{q^*+\delta}^{1/2} |b(q) - \varepsilon_q^W|^2 \, \mathrm{d}q.$$

For the first part, we notice that for $0 \leq q < q^* - \delta$, we have

$$b(q) < b(q^* - \delta) < b^* - \sigma < \varepsilon_q^W < \varepsilon_{q^*}^W = b^*.$$

This yields that

$$\forall\ 0 \leq q < q^* - \delta, \quad |b(q) - \varepsilon_q^W| = \varepsilon_q^W - b(q) < b^* - b(q) = |b(q) - b^*|.$$

Integrating this inequality leads to

$$\int_0^{q^*-\delta} |b(q) - \varepsilon_q^W|^2 \, \mathrm{d}q < \int_0^{q^*-\delta} |b(q) - b^*|^2 \, \mathrm{d}q.$$

Similarly, we obtain that

$$\int_{q^*+\delta}^{1/2} |b(q) - \varepsilon_q^W|^2 \, \mathrm{d}q < \int_{q^*+\delta}^{1/2} |b(q) - b^*|^2 \, \mathrm{d}q.$$

Lastly, for the middle part, we have

$$\int_{q^*-\delta}^{q^*+\delta} |b(q) - \varepsilon_q^W|^2 \, \mathrm{d}q < 2\delta \left[\varepsilon_{q^*+\delta}^W - \varepsilon_{q^*-\delta}^W\right] \leq 4\delta\sigma \leq \frac{\eta^{\mathrm{int}}}{2} < \int_{q^*-\delta}^{q^*+\delta} |b(q) - b^*|^2 \, \mathrm{d}q.$$

Combining all these inequalities yields that $\mathcal{J}_b(W) < \mathcal{K}_b(b^*)$. This contradicts the minimising character of the sequence $(V_n)_{n\in\mathbb{N}^*}$.

Hence the sequence $(\nu_n(\Gamma))_{n\in\mathbb{N}^*}$ is bounded. The proof of Theorem 2.3 then follows from Proposition 3.2.

4. Numerical tests

In this section, we present some numerical results obtained on different toy inverse band structure problems, which illustrates the theoretical results presented in Section 2.3.

In Section 4.1, we present the discretised version of the inverse band problem for multiple target bands. Numerical results on different test cases are given in Section 4.2. The reader should keep in mind that although the proof given in the previous section only works for the optimisation of the first band, it is possible to investigate cases where several bands are targeted from a numerical perspective.

4.1. Discretised inverse band structure problem

For $k \in \mathbb{Z}$, we let $e_k(x) := \frac{1}{\sqrt{2\pi}} e^{ikx}$ be the kth Fourier mode. For $s \in \mathbb{N}^*$, we define by

$$X_s := \mathrm{Span}\left\{e_k,\ k \in \mathbb{Z},\ |k| \leq s\right\} \tag{4.1}$$

the finite dimensional space of L^2_{per} consisting of the $N_s := 2s+1$ lowest Fourier modes. We denote by $\Pi_{X_s} : L^2_{\mathrm{per}} \to X_s$ the L^2_{per} orthogonal projector onto X_s. In practice, the solutions of the eigenvalue problem (2.4) are approximated using a Galerkin method in X_s. We denote by $\varepsilon^{V,s}_{q,1} \leq \cdots \leq \varepsilon^{V,s}_{q,N_s}$ the eigenvalues (ranked in increasing order, counting multiplicity) of the operator $A^{V,s}_q := \Pi_{X_s} A^V_q \Pi^*_{X_s}$. We also denote by $(u^{V,s}_{q,1}, \cdots, u^{V,s}_{q,N_s})$ an orthonormal basis of X_s composed of eigenvectors associated to these eigenvalues so that

$$\forall 1 \leq j \leq N_s, \quad A^{V,s}_q u^{V,s}_{q,j} = \varepsilon^{V,s}_{q,j} u^{V,s}_{q,j}. \tag{4.2}$$

An equivalent variational formulation of (4.2) is the following:

$$\forall 1 \leq j \leq N_s, \quad \forall v \in X_s, \quad a^V_q\left(u^{V,s}_{q,j}, v\right) = \varepsilon^{V,s}_{q,j} \left\langle u^{V,s}_{q,j}, v \right\rangle_{L^2_{\mathrm{per}}}.$$

As s goes to $+\infty$, we have $\varepsilon^{V,s}_{q,m} \underset{s\to+\infty}{\longrightarrow} \varepsilon^V_{q,m}$.

In order to perform the integration in (2.7), we discretise the Brillouin zone. We use a regular grid of size $Q \in \mathbb{N}^*$, and set

$$\Gamma^*_Q := \left\{-\frac{1}{2} + \frac{j}{Q},\ j \in \{0, \cdots, Q-1\}\right\}.$$

Since the maps $q \mapsto \varepsilon_{q,m}$ are analytic and periodic, the discretisation error coming from the integration will be exponentially small with respect to Q. In practice, we fix $Q \in \mathbb{N}^*$.

Let $M \in \mathbb{N}^*$ be a desired number of targeted bands and $b_1, \ldots, b_M \in C^0_{\mathrm{per}}$ be real-valued even functions, and such that b_m is increasing when m is odd and decreasing when m is even. Our cost functional is therefore $\mathcal{J}_Q : H^{-1}_{\mathrm{per},r} \to \mathbb{R}$, defined by

$$\forall V \in H^{-1}_{\mathrm{per,r}}, \quad \mathcal{J}_Q(V) := \frac{1}{Q} \sum_{q \in \Gamma^*_Q} \sum_{m=1}^{M} |b_m(q) - \varepsilon^V_{q,m}|^2.$$

Its discretised version, when the eigenvalues problems are solved with a Galerkin approximation, is

$$\forall s \in \mathbb{N}^*, \quad \forall V \in H^{-1}_{\mathrm{per,r}}, \quad \mathcal{J}^s_Q(V) := \frac{1}{Q} \sum_{q \in \Gamma^*_Q} \sum_{m=1}^{M} |b_m(q) - \varepsilon^{V,s}_{q,m}|^2.$$

Our goal is to find a potential $V \in H^{-1}_{\mathrm{per,r}}$ which minimise the functional $\mathcal{J}^s_Q$. In practice, an element $V \in H^{-1}_{\mathrm{per,r}}$ is approximated with a finite set of Fourier modes. For $p \in \mathbb{N}^*$, we denote by

$$Y_p := \mathrm{Span}\left\{ \sum_{k\in\mathbb{Z},\ |k|^2\leq p} \widehat{V}_k e_k,\ \forall k \in \mathbb{Z},\ |k| \leq p,\ \overline{\widehat{V}_{-k}} = \widehat{V}_k \right\}. \tag{4.3}$$

Altogether, we want to solve

$$V^{s,p} := \underset{V\in Y_p}{\arg\min}\, \mathcal{J}^s_Q(V). \tag{4.4}$$

For all $p \in \mathbb{N}^*$, $Y_p \subset \mathcal{C}^\infty_{\mathrm{per}}(-\pi,\pi)$, whereas the theoretical results presented in Section 2 suggest that the minimising potential should be sought in $H^{-1}_{\mathrm{per,r}}$. Actually, we expect that the choice of the parameter p in (4.4) might have a strong impact on solutions to (4.4), especially when the target bands b_m *are not* realisable bands. We illustrate this point in the second test case presented in Section 4.2.

To solve the minimisation problem (4.4), in all the numerical tests presented in Section 4.2, we use a quasi Newton with the Broyden-Fletcher-Goldfarb-Shanno formula (**BFGS**) algorithm [1].

The computation of the gradient of $\mathcal{J}^s_Q$ is done as follows. For all $V \in H^{-1}_{\mathrm{per,r}}$, there exists real-valued coefficients $\left(c^V_k\right)_{k\in\mathbb{N}}$ and $\left(d^V_k\right)_{k\in\mathbb{N}^*}$ such that

$$V(x) = c^V_0 + \sum_{k\in\mathbb{N}^*} c^V_k \cos(kx) + d^V_k \sin(kx), \qquad \text{and} \sum_{k\in\mathbb{N}^*} (1+|k|^2)^{-1}\left(|c^V_k|^2 + |d^V_k|^2\right) < +\infty.$$

For all $k \in \mathbb{N}$ (respectively $k \in \mathbb{N}^*$), we can express the derivative $\partial_{c^V_k}\mathcal{J}^s_Q(V)$ (respectively $\partial_{d^V_k}\mathcal{J}^s_Q(V)$) exactly in terms of the Bloch eigenvectors $u^{V,s}_{q,m}$. Indeed, it holds that

$$\partial_{c^V_k}\mathcal{J}^s_Q(V) = \frac{1}{Q}\sum_{q\in\Gamma^*_Q}\sum_{m=1}^{M} 2\left(\varepsilon^{V,s}_{q,m} - b_m(q)\right)\partial_{c^V_k}\left(\varepsilon^{V,s}_{q,m}\right).$$

On the other hand, from the Hellman-Feynman theorem, we have

$$\partial_{c^V_k}\left(\varepsilon^{V,s}_{q,m}\right) = \left\langle u^{V,s}_{q,m}, \partial_{c^V_k} A^V_q, u^{V,s}_{q,m}\right\rangle = \langle u^{V,s}_{q,m}, \cos(k\cdot)u^{V,s}_{q,m}\rangle_{L^2_{\mathrm{per}}}.$$

Similarly, for all $k \in \mathbb{N}^*$,

$$\partial_{d^V_k}\left(\varepsilon^{V,s}_{q,m}\right) = \left\langle u^{V,s}_{q,m}, \partial_{d^V_k} A^V_q, u^{V,s}_{q,m}\right\rangle = \langle u^{V,s}_{q,m}, \sin(k\cdot)u^{V,s}_{q,m}\rangle_{L^2_{\mathrm{per}}}.$$

4.2. Numerical results

In this section, we present some numerical results on the resolution of (4.4) obtained with the numerical procedure presented in Section 4.1.

4.2.1. Test case 1

We first present a numerical test case illustrating the difficulty of solving (4.4) due to the existence of multiple local minima in general.

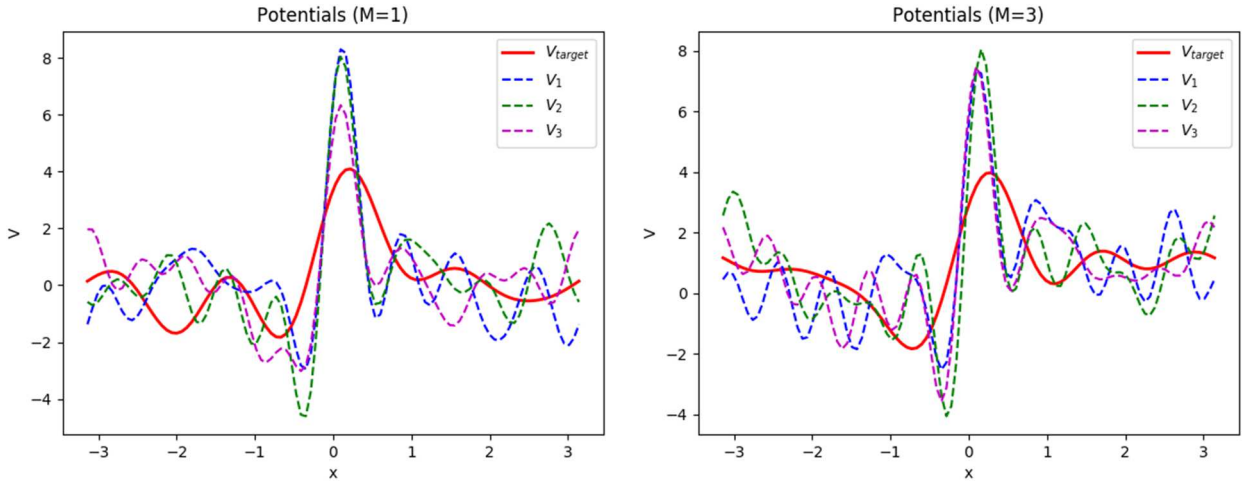

FIGURE 1. Potentials obtained at the end of the optimisation procedure, with different starting values. *Left*: Test case with $M = 1$; *Right*: Test case with $M = 3$.

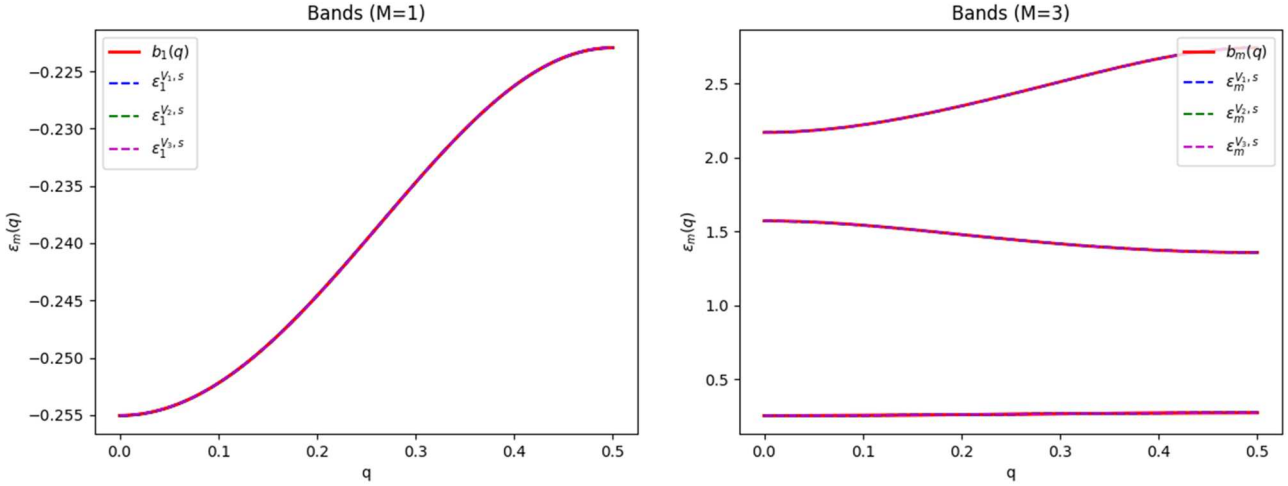

FIGURE 2. Bands obtained at the end of the optimisation procedure, with different starting values. *Left*: Test case with $M = 1$; *Right*: Test case with $M = 3$.

We set $p = 5$, $s = 20$ and $Q = 100$. A target potential V_{target} is chosen by sampling randomly the coefficients $\left(c_k^{V_{\text{target}}}\right)_{0\leq k\leq p}$ and $\left(d_k^{V_{\text{target}}}\right)_{1\leq k\leq p}$. The target bands $b_m(q)$ are defined as $b_m(q) := \varepsilon_{q,m}^{V_{\text{target}},s}$. We present numerical results in a first test case where $M = 1$, and in a second test case where $M = 3$.

In Figure 1, the potentials V_1, V_2 and V_3 obtained at the end of the optimisation procedure from three different starting values of the potential V (also chosen randomly) are plotted in dashed lines, and are to be compared with V_{target}, which is plotted in a full red line. The corresponding bands are plotted in Figure 2. Lastly, the evolution of the quantity $\sqrt{\mathcal{J}_Q^s}$ as a function of the number of iterations of the optimisation procedure is illustrated in Figure 3. From these plots, we can observe that V_1, V_2 and V_3 are quite different from V_{target} and from each other. Actually, these results numerically illustrate the fact that uniqueness of solutions to problem 4.4 cannot be expected due the isospectrality properties of one-dimensional Schrödinger operators (see Rem. 2.4).

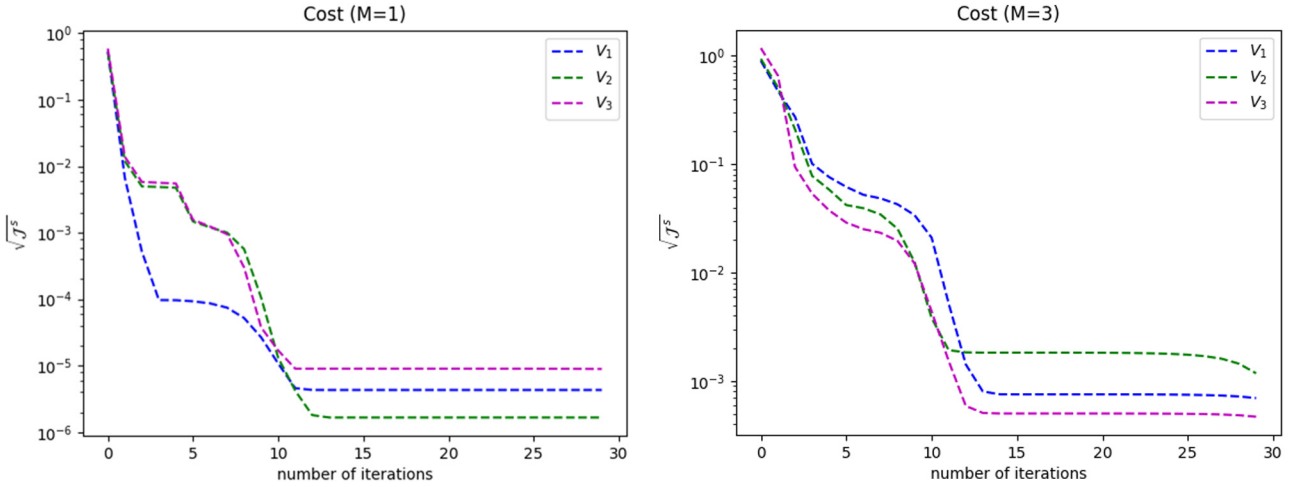

FIGURE 3. Evolution of the (square root of) cost as a function of the number of iterations in the optimisation procedure, with different starting values. *Left*: Test case with $M = 1$; *Right*: Test case with $M = 3$.

4.2.2. Test case 2 (Dirac band)

We give here an example which illustrates the need of considering singular potentials for the resolution of (4.4) in general. For $\lambda > 0$ and $q \in \Gamma^*$, we define $b_1(q) := \varepsilon_{q,1}^{V_{\nu_\lambda}}$ where

$$\nu_\lambda = \lambda \sum_{k \in 2\pi\mathbb{Z}} \delta_k,$$

Following similar calculations as for (3.5), we have $\varepsilon_{q,1}^{V_{\nu_\lambda}} = |\mu_\lambda(q)|^2$, where $\mu_\lambda(q) \in \mathbb{R}$ is solution to

$$\frac{\lambda}{2} \frac{\sin(2\pi\mu_\lambda(q))}{\mu_\lambda(q)} + \cos(2\pi\mu_\lambda(q)) = \cos(2\pi q).$$

For all $p \in \mathbb{N}^*$, we introduce a regularised potential $V_\lambda^p \in Y_p$ defined by

$$\forall x \in (-\pi, \pi), \quad V_\lambda^p(x) := \lambda \sum_{|k| \leq p} e^{i2\pi kx},$$

so that $V_\lambda^p \underset{p \to +\infty}{\longrightarrow} V_{\nu_\lambda}$ in $H^{-1}_{\mathrm{per,r}}$. We also denote by $\widetilde{V}_\lambda^p \in Y^p$ the potential obtained by a BFGS optimisation procedure when optimising $\mathcal{J}_Q^s$ over the set Y_p from the initial guess V_λ^p.

In the numerical tests presented above, $\lambda = 10$, $Q = 100$ and $s = 60$. Two curves are plotted in Figure 4. The first curve (in dashed line) represents the value of $\sqrt{\mathcal{J}_Q^s(V_\lambda^p)}$ for different values of p. The second curve (in full line) represents the value $\sqrt{\mathcal{J}_Q^s(\widetilde{V}_\lambda^p)}$. Figure 5 shown the potentials obtained by this procedure for different values of p along with their associated first band.

From these plots, we clearly see that the quality of approximation of the target band $b_1(q)$ strongly depends on the choice of the parameter p, and, naturally, the larger p, the better the accuracy of the approximation.

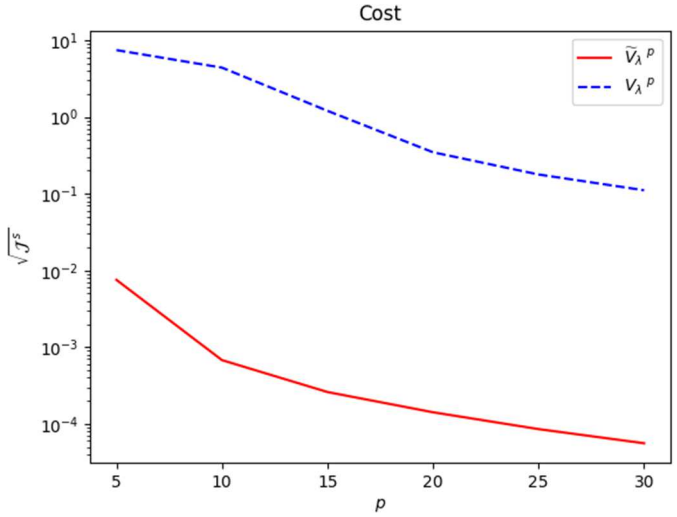

FIGURE 4. Evolution of $\sqrt{\mathcal{J}_Q^s\,(V_\lambda^p)}$ and of $\sqrt{\mathcal{J}_Q^s(\widetilde{V}_\lambda^p)}$ as a function of p.

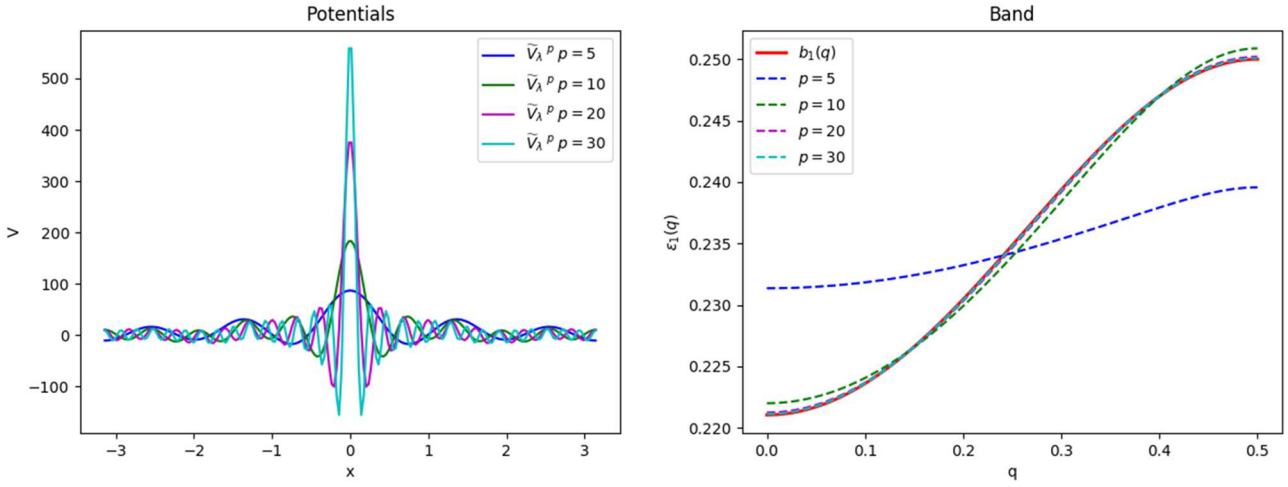

FIGURE 5. Potentials and bands obtained at the end of the optimisation procedure, for different values of p.

4.2.3. Test case 3 (flat band)

We give here numerical results on a test case where $M = 1$ and where the target band $b_1(q)$ *cannot* be the first band of a potential. We choose b_1 to be a *flat band*, *i.e.* $b_1(q) = 0$. We set here $p = 10$ and $s = 20$. We start from an initial potential which is a small random perturbation of the zero potential. In Figure 6, are plotted the obtained potentials after $n_{it} = 10$, 20 and 30 iterations of the optimisation procedure, along with their corresponding bands. The evolutions of the (square root of the) cost and of the L^1 norm of the obtained potential as a function of the number of iterations of the optimisation procedure are plotted in Figure 7. We observe that, in agreement with Proposition 2.5, the L^1 norm of the potential steadily increases as the number of iterations of the optimisation algorithm grows.

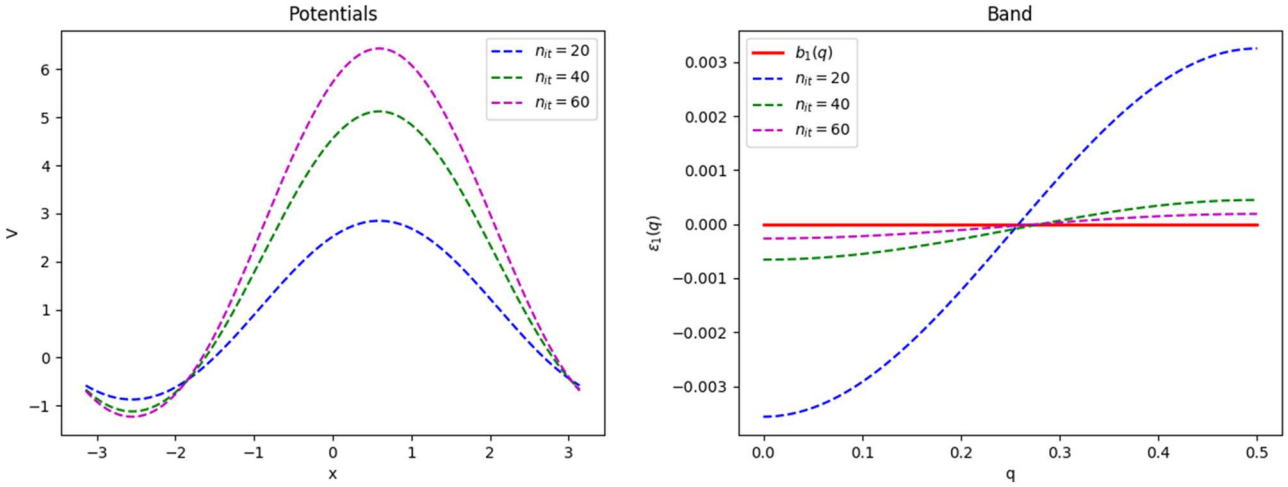

FIGURE 6. Flat target band: potentials (*left*) and bands (*right*) obtained after $n_{it} = 20, 40, 60$ iterations of the optimisation procedure.

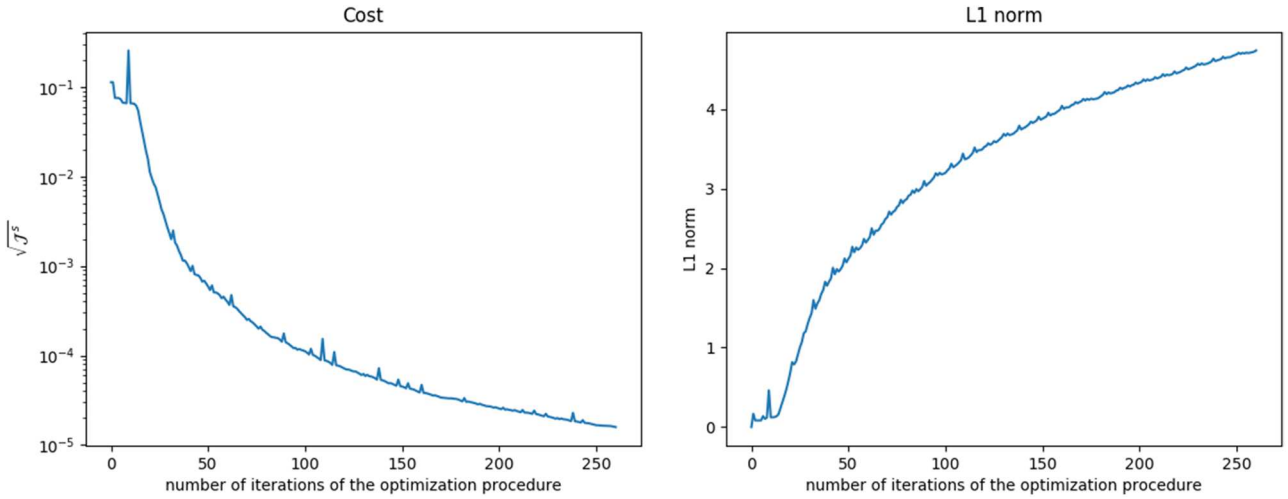

FIGURE 7. Flat target band: evolution of the cost (*left*) and of the L^1 norm of the potential (*right*) as a function of the number of iterations in the optimisation procedure.

5. Conclusion

This work focuses on the theoretical analysis of a least-square minimisation problem for the optimisation of the first band(s) in an inverse Hill's problem. The theoretical and numerical results indicate that it is necessary to consider a class of singular potentials for the considered optimisation problem to have at least one solution. An interesting perspective of research is the development of new numerical approaches in order to allow the manipulation of singular potentials also on the discrete level. For instance, the number of Fourier modes used to discretise the potential could be adapted in an appropriate way along the iteration of the optimisation procedure.

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