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DISCRETE BETHE-SOMMERFELD CONJECTURE

RUI HAN AND SVETLANA JITOMIRSKAYA

ABSTRACT. In this paper, we prove a discrete version of the Bethe-Sommerfeld conjecture. Namely, we show that the spectra of multi-dimensional discrete periodic Schrödinger operators on $\mathbb{Z}^d$ lattice with sufficiently small potentials contain at most two intervals. Moreover, the spectrum is a single interval, provided one of the periods is odd, and can have a gap whenever all periods are even.

1. Introduction

Bethe-Sommerfeld conjecture states that for $d \geq 2$ and any periodic function $V : \mathbb{R}^d \to \mathbb{R}$, the spectrum of the continuous Schrödinger operator:

$$-\Delta + V$$

contains only finitely many gaps, so no gaps for large energies. This conjecture has been studied extensively with many important advances [1, 3, 4, 7, 8, 9, 10, 11, 12]. Finally, Parnovski [6], proved it in any dimension $d \geq 2$, under smoothness conditions on the potential V (see [13] for an alternative approach).

In this paper, we consider a discrete version of this conjecture. A discrete multi-dimensional periodic Schrödinger operator on $l^2(\mathbb{Z}^d)$ is given by:

$$(H_V u)(\boldsymbol{n}) = \sum_{|\boldsymbol{m}-\boldsymbol{n}|=1} u(\boldsymbol{m}) + V(\boldsymbol{n})u(\boldsymbol{n}), \tag{1.1}$$

where $|\boldsymbol{m}-\boldsymbol{n}| = \sum_{i=1}^d |m_i - n_i|$. We assume $V(\cdot)$ is a bounded real-valued periodic function on $\mathbb{Z}^d$ with period $\boldsymbol{q} = (q_1, q_2, ..., q_d)$, namely, $V(\boldsymbol{n} + q_i \boldsymbol{b}_i) = V(\boldsymbol{n})$, with $\{\boldsymbol{b}_i\}_{i=1}^d$ being the standard basis for $\mathbb{R}^d$. [1].In the high energy regime continuous Schrödinger operators can be viewed as perturbations of the free Laplacian. In this sense the proper discrete analogy of the Bethe-Sommerfeld conjecture is absence of gaps for small coupling discrete periodic operators.

The discrete Bethe-Sommerfeld conjecture has been proved for $d = 2$ by Embree-Fillman [2], with a partial result (for coprime periods) earlier by Krüger [5]. The approach of [2] runs into combinatorial/algebraic difficulties for $d > 2$. Here we prove this conjecture for arbitrary dimensions:

Theorem 1.1. *Let $d \geq 2$ and a period $\boldsymbol{q} = (q_1, q_2, ..., q_d)$ be given. There exists a constant $c_{\boldsymbol{q}} > 0$ such that the following statements hold:*

1. *If $\|V\|_\infty \leq c_{\boldsymbol{q}}$, then the spectrum of H_V contains at most two intervals.*
2. *If at least one of q_i is odd, and $\|V\|_\infty \leq c_{\boldsymbol{q}}$, then the spectrum of H_V is a single interval.*

Our result is sharp in the sense that if all the q_i's are even, then there exists V (see example in Section 6) with *minimal period* $\boldsymbol{q}$, and arbitrarily small $\|V\|_\infty$ such that $\Sigma(H_V)$ contains *exactly* two intervals. The example we give is a modification of Krüger's example [5], in which $V(\boldsymbol{n}) = \delta(-1)^{|\boldsymbol{n}|}$

[1]The most general periodic case may seem to be $V(\boldsymbol{n} + \boldsymbol{w}_i) = V(\boldsymbol{n})$, where $\boldsymbol{w}_i \in \mathbb{Z}^d$, $i = 1, ..., d$, are linearly independent vectors. This however reduces toour assumption because such operators are periodic with period $\boldsymbol{q} = (\det W, ..., \det W)$, where W is the matrix with $\boldsymbol{w}_i$ as columns.

has minimal period $(2, 2, ..., 2)$. Also it is well-known that both $d \geq 2$ and the smallness of $\|V\|_\infty$ are needed.

The strategy of our proof relies on analysing the overlaps of adjacent bands of the spectrum. We refer the readers to [5] for detailed background on discrete multi-dimensional Schrödinger operators. Here we only introduce some notations and known results. Let us denote the spectrum of H by $\Sigma(H)$. By Floquet-Bloch decomposition, $\Sigma(H_V)$ can be decomposed into $\cup_{\boldsymbol{\theta}\in\Theta}\Sigma(H_V^{\boldsymbol{\theta}})$, where $\Theta = \{\boldsymbol{\theta} = (\theta_1, \theta_2, ..., \theta_d) : 0 \leq \theta_i < \frac{1}{q_i},\ 1 \leq i \leq d\}$ is a d-dimensional torus (by gluing 0 and $\frac{1}{q_i}$ together in the $\boldsymbol{b}_i$ direction), and $H_V^{\boldsymbol{\theta}}$ is the periodic Schrödinger operator with the following boundary condition:

$$u_{\boldsymbol{n}+q_i\boldsymbol{b}_i} = e^{2\pi i q_i\theta_i}u_{\boldsymbol{n}}.$$

Each operator $H_V^{\boldsymbol{\theta}}$ clearly has $Q = \prod_{i=1}^d q_i$ eigenvalues, which we will order in the *decreasing* order and denote them by $E_V^1(\boldsymbol{\theta}) \geq E_V^2(\boldsymbol{\theta}) \geq \cdots \geq E_V^Q(\boldsymbol{\theta})$. Let $F_V^k = \cup_{\boldsymbol{\theta}\in\Theta}E_V^k(\boldsymbol{\theta})$ be the k-th band of the spectrum. Theorem 1.1 is thus reduced to proving non-empty overlaps of arbitrary two adjacent bands, with only possible exception around the point 0. Employing a standard perturbation argument (see Theorem 3.1), this is made possible via proving non-empty overlaps of the *interiors* of adjacent bands of the free Laplacian H_0. Two of our key lemmas are as follows:

Lemma 1.2. *If $E \in (-2d, 2d) \setminus \{0\}$, then $E \in \mathrm{int}(F_0^k)$ for some $1 \leq k \leq Q$.*

Lemma 1.3. *If at least one of q_i's is odd, then $0 \in \mathrm{int}(F_0^k)$ for some $1 \leq k \leq Q$.*

We will prove Lemma 1.2 in Section 4 and Lemma 1.3 in Section 5. Different from the existing $d = 2$ proofs in [5, 2], our argument proceeds by contradiction. Namely we assume $E_0^{k_0}(\tilde{\theta}) = \min F_0^{k_0} = \max F_0^{k_0+1}$ for certain k_0, and then apply a novel *perturb-and-count* technique. We perturb the phase $\tilde{\theta}$ and count the number of eigenvalues that move up and down. It is then argued that different chosen directions lead to different numbers of eigenvalues that go up/down, hence a contradiction.

2. Preliminaries

For $\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}} \in \Theta$, let $\|\boldsymbol{\theta} - \tilde{\boldsymbol{\theta}}\|_\Theta$ be the torus distance between them, defined by

$$\|\boldsymbol{\theta} - \tilde{\boldsymbol{\theta}}\|_\Theta^2 = \sum_{i=1}^d \|\theta_i - \tilde{\theta}_i\|_{\mathbb{T}_i}^2,$$

where $\|\theta\|_{\mathbb{T}_i} := \mathrm{dist}(\theta, \frac{1}{q_i}\mathbb{Z})$.

2.1. Spectrum of the free Laplacian.

It is a well-known result that the spectrum of the free Laplacian H_0 is a whole interval:

$$\Sigma(H_0) = [-2d, 2d]. \tag{2.1}$$

By Floquet-Bloch decomposition,

$$\Sigma(H_0) = [-2d, 2d] = \cup_{\boldsymbol{\theta}\in\Theta}\Sigma(H_0^{\boldsymbol{\theta}}). \tag{2.2}$$

Furthermore, each $\Sigma(H_0^{\boldsymbol{\theta}})$ can be written down explicitly,

$$\Sigma(H_0^{\boldsymbol{\theta}}) = \left\{ e_0^{\boldsymbol{l}}(\boldsymbol{\theta}) := 2\sum_{i=1}^d \cos 2\pi(\theta_i + \frac{l_i}{q_i}) \right\}_{\boldsymbol{l}\in\Lambda}, \tag{2.3}$$

where $\Lambda = \{\boldsymbol{l} = (l_1, l_2, ..., l_d) : 0 \leq l_i \leq q_i - 1,\ 1 \leq i \leq d\}$.

3. Proof of Theorem 1.1

We say the bands $\{F_k\}_{k=1}^Q$ of H are δ-overlapping if $\max F^{k+1} - \min F^k \geq \delta$ for any $1 \leq k \leq Q-1$. Theorem 1.1 follows from a quick combination of Lemmas 1.2, 1.3 with Hausdorff continuity of the spectrum. The form of continuity convenient to us is presented in:

Theorem 3.1. *([5], Theorem 3.8) Let the bands of H be δ-overlapping. Then the bands of $H+V$ are $\delta - 2\|V\|_\infty$-overlapping.*

□

4. Proof of Lemma 1.2

Our strategy is to prove by contradiction, namely we assume $\min F_0^{k_0} = \max F_0^{k_0+1} \neq 0$ for some $1 \leq k_0 \leq Q$ and try to get a contradiction. Without loss of generality, we assume $\min F_0^{k_0} = \max F_0^{k_0+1} > 0$.

We will use the following elementary lemma, whose proof will be included in the appendix.

Lemma 4.1. *Let $d \geq 2$. For any $E \in (-2d, 2d)$, there exists $\boldsymbol{\theta} = (\theta_1, \theta_2, ..., \theta_d)$ with $\theta_i \in [0,1)$ such that*

$$\begin{cases} \sum_{i=1}^d 2\cos 2\pi\theta_i = E, \\ \sum_{i=1}^d \sin 2\pi\theta_i = 0, \\ \sum_{i=1}^d \sin^2 2\pi\theta_i \neq 0. \end{cases}$$

Now let us prove Lemma 1.2.

First, by Lemma 4.1, there exists $\tilde{\boldsymbol{\theta}} = (\tilde{\theta}_1, \tilde{\theta}_2, ..., \tilde{\theta}_d) \in \Theta$ and $\boldsymbol{l}^{(1)} = (l_1^{(1)}, l_2^{(1)}, ..., l_d^{(1)}) \in \Lambda$ such that

$$\begin{cases} \min F_0^{k_0} = \sum_{i=1}^d 2\cos 2\pi(\tilde{\theta}_i + \frac{l^{(1)}}{q_i}) = e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}), \\ 0 = \sum_{i=1}^d \sin 2\pi(\tilde{\theta}_i + \frac{l^{(1)}}{q_i}), \\ 0 \neq \sum_{i=1}^d \sin^2 2\pi(\tilde{\theta}_i + \frac{l^{(1)}}{q_i}). \end{cases} \tag{4.1}$$

Next, let us choose $\boldsymbol{l}^{(2)}, \boldsymbol{l}^{(3)}, ..., \boldsymbol{l}^{(r)} \in \Lambda$ (if any) be *all* the vectors in Λ such that

$$e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}) = e_0^{\boldsymbol{l}^{(2)}}(\tilde{\boldsymbol{\theta}}) = \cdots = e_0^{\boldsymbol{l}^{(r)}}(\tilde{\boldsymbol{\theta}}).$$

Then clearly they are $E_0^{k_0-s}(\tilde{\boldsymbol{\theta}}) = \cdots = E_0^{k_0}(\tilde{\boldsymbol{\theta}}) = \cdots = E_0^{k_0+r-s-1}(\tilde{\boldsymbol{\theta}})$, for some $0 \leq s \leq r-1$. And also we have $E_0^{k_0-s-1}(\tilde{\boldsymbol{\theta}}) > E_0^{k_0-s}(\tilde{\boldsymbol{\theta}})$, $E_0^{k_0+r-s-1}(\tilde{\boldsymbol{\theta}}) > E_0^{k_0+r-s}(\tilde{\boldsymbol{\theta}})$. By the continuity of each eigenvalue, we could choose $\epsilon > 0$ small enough, such that for any $\|\boldsymbol{\theta} - \tilde{\boldsymbol{\theta}}\|_\Theta < \epsilon$, we always have

$$E_0^{k_0-s-1}(\boldsymbol{\theta}) > E_0^{k_0-s}(\boldsymbol{\theta}) \text{ and } E_0^{k_0+r-s-1}(\boldsymbol{\theta}) > E_0^{k_0+r-s}(\boldsymbol{\theta}). \tag{4.2}$$

Let $J_0 \geq 0$ be the number of j's such that $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \mathbf{0}$. For $\boldsymbol{\beta} \in \mathbb{R}^d$, we also introduce $J_{\boldsymbol{\beta}}$ and $J_{\boldsymbol{\beta}}^0$: let $J_{\boldsymbol{\beta}}$ be the number of j's such that $\boldsymbol{\beta} \cdot \nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) > 0$, and $J_{\boldsymbol{\beta}}^0$ be the number of j's such that $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) \neq \mathbf{0}$ and $\boldsymbol{\beta} \cdot \nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = 0$.

Perturbing $e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}})$ along the direction of $\boldsymbol{\beta}$ we get:

$$e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}) = e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + t\boldsymbol{\beta}\cdot\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + O(t^2) \tag{4.3}$$

$$= e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + t\boldsymbol{\beta}\cdot\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + \frac{t^2}{2}\left(-4\pi^2\sum_{i=1}^{d} 2\cos 2\pi(\tilde{\theta}_i + \frac{l_i^{(j)}}{q_i})\beta_i^2\right) + O(t^3). \tag{4.4}$$

Step 1.

Let $\tilde{\boldsymbol{\beta}} = \frac{1}{\sqrt{d}}(1,1,...,1)$. By (4.1), we have

$$\tilde{\boldsymbol{\beta}}\cdot\nabla e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}) = 0 \ \text{ and } \ \nabla e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}) \neq \mathbf{0}, \tag{4.5}$$

which implies $J_{\tilde{\boldsymbol{\beta}}}^0 \geq 1$.

By (4.4) for j such that $\tilde{\boldsymbol{\beta}}\cdot\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = 0$ (in total $J_0 + J_{\tilde{\boldsymbol{\beta}}}^0$ many such j's), we have

$$e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) = (1-\frac{2\pi^2}{d}t^2)e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + O(t^3) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}), \tag{4.6}$$

for $|t|$ small enough. Let us mention that in (4.6), we used the fact that $e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \min F_0^{k_0} > 0$.

Now combine (4.3) with (4.6). On one hand, we have, for $\epsilon > t > 0$ small enough,

- there are $J_{\tilde{\boldsymbol{\beta}}}$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \max F_0^{k_0+1}$, thus $J_{\tilde{\boldsymbol{\beta}}} \leq (k_0+1)-(k_0-s-1)-1 = s+1$.
- for the other $r - J_{\tilde{\boldsymbol{\beta}}}$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \min F_0^{k_0}$, so $r - J_{\tilde{\boldsymbol{\beta}}} \leq (k_0+r-s-1)-(k_0+1)+1 = r-s-1$.

Thus

$$J_{\tilde{\boldsymbol{\beta}}} = s+1. \tag{4.7}$$

On the other hand, for $0 > t > -\epsilon$ small enough, we have,

- there are $r - J_{\tilde{\boldsymbol{\beta}}} - J_{\tilde{\boldsymbol{\beta}}}^0 - J_0$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \max F_0^{k_0+1}$,
- for the other $J_{\tilde{\boldsymbol{\beta}}} + J_{\tilde{\boldsymbol{\beta}}}^0 + J_0$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\tilde{\boldsymbol{\beta}}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \min F_0^{k_0}$.

Thus

$$J_{\tilde{\boldsymbol{\beta}}} + J_{\tilde{\boldsymbol{\beta}}}^0 + J_0 = r-s-1. \tag{4.8}$$

Combining this with (4.7), we have,

$$r - 2s = J_{\tilde{\boldsymbol{\beta}}}^0 + J_0 + 2. \tag{4.9}$$

Step 2.

We choose $\boldsymbol{\beta} \in \mathbb{R}^d$, $\|\boldsymbol{\beta}\|_{\mathbb{R}^d} = 1$, such that $\boldsymbol{\beta}\cdot\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) \neq 0$ for any $1 \leq j \leq r$ with $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) \neq \mathbf{0}$, and satisfies the following:

$$\sum_{i=1}^{d} 2|\beta_i^2 - \frac{1}{d}| < \frac{1}{2d}\min F_0^{k_0}. \tag{4.10}$$

Inequality (4.10) basically says $\boldsymbol{\beta} \sim \tilde{\boldsymbol{\beta}}$.

For j such that $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \mathbf{0}$, we have, by (4.4),(4.10)

$$e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) = e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + \frac{t^2}{2}\left(-\frac{4\pi^2}{d}e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + 4\pi^2\sum_{i=1}^{d} 2\cos 2\pi(\tilde{\theta}_i + \frac{l_i^{(j)}}{q_i})(\frac{1}{d} - \beta_i^2)\right) + O(t^3)$$

$$\leq (1 - \frac{\pi^2}{d}t^2)e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + O(t^3) \tag{4.11}$$

$$< e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}). \tag{4.12}$$

Combining (4.3) with (4.12), on one hand, we have that for $\epsilon > t > 0$ small enough,

- there are $J_{\boldsymbol{\beta}}$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \max F_0^{k_0+1}$,
- for the other $r - J_{\boldsymbol{\beta}}$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \min F_0^{k_0}$.

Thus

$$J_{\boldsymbol{\beta}} = s + 1. \tag{4.13}$$

On the other hand, we have that for $0 > t > -\epsilon$ small enough,

- there are $r - J_{\boldsymbol{\beta}} - J_0$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \max F_0^{k_0+1}$,
- for the other $J_{\boldsymbol{\beta}} + J_0$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \min F_0^{k_0}$.

Thus

$$J_{\boldsymbol{\beta}} + J_0 = r - s - 1. \tag{4.14}$$

Combining this with (4.13), we have,

$$r - 2s = J_0 + 2. \tag{4.15}$$

However, this contradicts with (4.9), since $J_{\tilde{\boldsymbol{\beta}}}^0 \geq 1$. □

5. Proof of Lemma 1.3

The spirit of this proof is similar to that of Lemma 1.2, but requires different choices of $\tilde{\boldsymbol{\theta}}, \boldsymbol{l}^{(1)}$ and $\boldsymbol{\beta}, \tilde{\boldsymbol{\beta}}$.

Without loss of generality, we assume q_1 is odd. We assume q_i's, $i \geq 2$, are even, since otherwise, we could simply replace q_i with $2q_i$, $i \geq 2$. Throughout this section, we will consider the case when $\min F_0^{k_0} = \max F^{k_0+1} = 0$.

5.1. $d = 2$.

This result has already been proved in [2]. Here we give an alternative self-contained proof.

We let $\tilde{\boldsymbol{\theta}} = (\frac{1}{2q_1}, 0)$, $\boldsymbol{l}^{(1)} = (\frac{q_1-1}{2}, 0)$, and observe that

$$\begin{cases} 0 = 2\cos\pi + 2\cos 0 = e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}), \\ \mathbf{0} = \nabla e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}). \end{cases} \tag{5.1}$$

Again, we let $\boldsymbol{l}^{(2)}, ..., \boldsymbol{l}^{(r)} \in \Lambda$ (if any) to be *all* the vectors in Λ such that $e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}) = e_0^{\boldsymbol{l}^{(2)}}(\tilde{\boldsymbol{\theta}}) = \cdots = e_0^{\boldsymbol{l}^{(r)}}(\tilde{\boldsymbol{\theta}}) = 0$. Let $0 \leq s \leq r - 1$ be such that $E_0^{k_0-s-1}(\boldsymbol{\theta}) > E_0^{k_0-s}(\boldsymbol{\theta}) = \cdots = E_0^{k_0}(\boldsymbol{\theta}) = \cdots = E_0^{k_0+r-s-1}(\boldsymbol{\theta}) > E_0^{k_0+r-s}(\boldsymbol{\theta})$ for any $\|\boldsymbol{\theta} - \tilde{\boldsymbol{\theta}}\|_\Theta < \epsilon$.

Let $\boldsymbol{l}^{(j)}$, $1 \leq j \leq r$, be such that $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \mathbf{0}$. Then $\sin 2\pi(\tilde{\theta}_1 + \frac{l_1^{(j)}}{q_1}) = \sin 2\pi(\tilde{\theta}_2 + \frac{l_2^{(j)}}{q_2}) = 0$. Taking into account that $e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = 0$, this implies $j = 1$. Hence the number of j's such that $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \mathbf{0}$ is equal to 1.

Now let $\boldsymbol{\beta}^+ = (1, 0)$ and $\boldsymbol{\beta}^- = (0, 1)$. Let $J_{\boldsymbol{\beta}^\pm}$, $J_{\boldsymbol{\beta}^\pm}^0$ be as in the proof of Lemma 1.2.

First, it is easy to see that $J^0_{\boldsymbol{\beta}^+}=J^0_{\boldsymbol{\beta}^-}=0$. Indeed, if there is j such that $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}})\neq \mathbf{0}$ and $\boldsymbol{\beta}^+\cdot\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}})=0$, then $\sin 2\pi(\tilde{\theta}_1+\frac{l_1^{(j)}}{q_1})=0$, which implies $\cos 2\pi(\tilde{\theta}_1+\frac{l_1^{(j)}}{q_1})=\pm 1$. This in turn implies $\cos 2\pi(\tilde{\theta}_2+\frac{l_2^{(j)}}{q_2})=\mp 1$, and hence $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}})=\mathbf{0}$, contradiction. The case $J^0_{\boldsymbol{\beta}^-}=0$ can be argued in the same way.

Secondly, by (4.4), we have that for $|t|<\epsilon$ small enough,

$$e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^{\pm})=\pm\, 4\pi^2t^2+O(t^3), \tag{5.2}$$

so $e_0^{\boldsymbol{l}^{(1)}}$ increases in the direction of $\boldsymbol{\beta}^+$ and decreases in the direction of $\boldsymbol{\beta}^-$.

Combining (4.3) with (5.2) for $\boldsymbol{\beta}^+$, on one hand, we have, for $\epsilon>t>0$ small enough,

- there are $J_{\boldsymbol{\beta}^+}+1$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)>e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)>0=\max F_0^{k_0+1}$,
- for the other $r-J_{\boldsymbol{\beta}^+}-1$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)<e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)<0=\min F_0^{k_0}$.

Hence

$$J_{\boldsymbol{\beta}^+}+1=s+1. \tag{5.3}$$

On the other hand, for $0>t>-\epsilon$ small enough, we have,

- there are $r-J_{\boldsymbol{\beta}^+}$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)>e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)>0=\max F_0^{k_0+1}$,
- for the other $J_{\boldsymbol{\beta}^+}$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)<e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^+)<0=\min F_0^{k_0}$.

Hence

$$J_{\boldsymbol{\beta}^+}=r-s-1. \tag{5.4}$$

Thus combining (5.3) with (5.4), we have

$$r=2s+1. \tag{5.5}$$

Similarly, combining (4.3) with (5.2) for $\boldsymbol{\beta}^-$, on one hand, we have, for $\epsilon>t>0$ small enough,

- there are $J_{\boldsymbol{\beta}^-}$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)>e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)>0=\max F_0^{k_0+1}$,
- for the other $r-J_{\boldsymbol{\beta}^-}$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)<e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)<0=\min F_0^{k_0}$.

Hence

$$J_{\boldsymbol{\beta}^-}=s+1. \tag{5.6}$$

On the other hand, for $0>t>-\epsilon$ small enough, we have,

- there are $r-J_{\boldsymbol{\beta}^-}-1$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)>e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)>0=\max F_0^{k_0+1}$,
- for the other $J_{\boldsymbol{\beta}^-}+1$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)<e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}+t\boldsymbol{\beta}^-)<0=\min F_0^{k_0}$.

Hence

$$J_{\boldsymbol{\beta}^-}+1=r-s-1. \tag{5.7}$$

Thus combining (5.6) with (5.7), we have

$$r=2s+3. \tag{5.8}$$

This contradicts with (5.5). □

5.2. $d \geq 3$.

Let us choose $\tilde{\boldsymbol{\theta}}, \boldsymbol{l}^{(1)}$ with $\tilde{\theta}_1 = \frac{1}{2q_1}, l_1^{(1)} = \frac{q_1-1}{2}$ and $\tilde{\theta}_i, l_i^{(1)}, 2 \leq i \leq d$, be such that $\cos 2\pi(\tilde{\theta}_i + \frac{l_i^{(1)}}{q_i}) = \frac{1}{d-1} < 1$ and $\sin 2\pi(\tilde{\theta}_i + \frac{l_i^{(1)}}{q_i}) > 0$. Let $\boldsymbol{\beta} = (1, 0, 0, ..., 0)$, then clearly we have,

$$\nabla e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}) \neq \mathbf{0} \quad \text{and} \quad \boldsymbol{\beta} \cdot \nabla e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}) = 0. \tag{5.9}$$

Let $\boldsymbol{l}^{(2)}, ..., \boldsymbol{l}^{(r)} \in \Lambda$ (if any) be *all* the vectors in Λ such that $e_0^{\boldsymbol{l}^{(1)}}(\tilde{\boldsymbol{\theta}}) = e_0^{\boldsymbol{l}^{(2)}}(\tilde{\boldsymbol{\theta}}) = \cdots = e_0^{\boldsymbol{l}^{(r)}}(\tilde{\boldsymbol{\theta}})$. Let $0 \leq s \leq r-1$ be such that $E_0^{k_0-s-1}(\boldsymbol{\theta}) > E_0^{k_0-s}(\boldsymbol{\theta}) = \cdots = E_0^{k_0}(\boldsymbol{\theta}) = \cdots = E_0^{k_0+r-s-1}(\boldsymbol{\theta}) > E_0^{k_0+r-s}(\boldsymbol{\theta})$ for any $\|\boldsymbol{\theta} - \tilde{\boldsymbol{\theta}}\|_\Theta < \epsilon$.

Let J_0, $J_{\boldsymbol{\beta}}$, $J_{\boldsymbol{\beta}}^0$ be as in the proof of Lemma 1.2. Then by (5.9), $J_{\boldsymbol{\beta}}^0 \geq 1$.

Clearly, for $J_0 + J_{\boldsymbol{\beta}}^0$ many j's, we have $\boldsymbol{\beta} \cdot \nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = 0$, which means $\sin 2\pi(\tilde{\theta}_1 + \frac{l_1^{(j)}}{q_1}) = 0$. Since our $\tilde{\theta}_1$ equals $\frac{1}{2q_1}$, we must have

$$\cos 2\pi(\tilde{\theta}_1 + \frac{l_1^{(j)}}{q_1}) = -1. \tag{5.10}$$

Thus, by (4.4) and (5.10), we have that for j (in total $J_0 + J_{\boldsymbol{\beta}}^0$ many) such that $\boldsymbol{\beta} \cdot \nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = 0$, for $|t| < \epsilon$ small enough,

$$\begin{aligned} e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) =& e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) + \frac{t^2}{2}\left(-8\pi^2 \cos 2\pi(\tilde{\theta}_1 + \frac{l_1^{(j)}}{q_1})\right) + O(t^3) \\ =& 4\pi^2 t^2 + O(t^3) \\ >& 0. \end{aligned} \tag{5.11}$$

Hence, combining (4.3) with (5.11), on one hand, we have, for $\epsilon > t > 0$ small enough,

- there are $J_{\boldsymbol{\beta}} + J_0 + J_{\boldsymbol{\beta}}^0$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > 0 = \max F_0^{k_0+1}$,
- for the other $r - J_{\boldsymbol{\beta}} - J_0 - J_{\boldsymbol{\beta}}^0$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < 0 = \min F_0^{k_0}$.

Hence

$$J_{\boldsymbol{\beta}} + J_0 + J_{\boldsymbol{\beta}}^0 = s + 1. \tag{5.12}$$

On the other hand, for $0 > t > -\epsilon$ small enough, we have,

- there are $r - J_{\boldsymbol{\beta}}$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) > 0 = \max F_0^{k_0+1}$,
- for the other $J_{\boldsymbol{\beta}}$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\boldsymbol{\beta}) < 0 = \min F_0^{k_0}$.

Hence

$$J_{\boldsymbol{\beta}} = r - s - 1. \tag{5.13}$$

Thus combining (5.3) with (5.4), we have

$$2s - r = J_0 + J_{\boldsymbol{\beta}}^0 - 2. \tag{5.14}$$

Now we choose $\tilde{\boldsymbol{\beta}} \in \mathbb{R}^d$, $\|\tilde{\boldsymbol{\beta}}\|_{\mathbb{R}^d} = 1$, such that $\tilde{\boldsymbol{\beta}} \cdot \nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) \neq 0$ for any $1 \leq j \leq r$ with $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) \neq \mathbf{0}$, and satisfies the following:

$$1 - \tilde{\beta}_1^2 + \sum_{i=2}^d \tilde{\beta}_i^2 < \frac{1}{2}. \tag{5.15}$$

This inequality essentially says $\tilde{\boldsymbol{\beta}} \sim \boldsymbol{\beta}$.

With $J_{\tilde{\boldsymbol{\beta}}}$ defined as before, by (4.4), (5.10) and (5.15), we have that for j (in total J_0 many) such that $\nabla e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}}) = \mathbf{0}$, for $|t| < \epsilon$ small enough,

$$\begin{aligned} e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) =& \frac{t^2}{2}\left(8\pi^2 - 8\pi^2(1-\tilde{\beta}_1^2) - 8\pi^2\sum_{i=2}^{d}\cos 2\pi(\tilde{\theta}_i + \frac{l_i^{(j)}}{q_i})\tilde{\beta}_i^2\right) + O(t^3) \\ >& 2\pi^2 t^2 + O(t^3) > 0. \end{aligned} \tag{5.16}$$

As before, combining (4.3) with (5.16), on one hand, we have, for $\epsilon > t > 0$ small enough,

- there are $J_0 + J_{\tilde{\boldsymbol{\beta}}}$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) > 0 = \max F_0^{k_0+1}$,
- for the other $r - J_0 - J_{\tilde{\boldsymbol{\beta}}}$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) < 0 = \min F_0^{k_0}$.

Hence

$$J_0 + J_{\tilde{\boldsymbol{\beta}}} = s + 1. \tag{5.17}$$

On the other hand, for $0 > t > -\epsilon$ small enough, we have,

- there are $r - J_{\tilde{\boldsymbol{\beta}}}$ many j's such that $E^{k_0-s-1}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) > e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) > 0 = \max F_0^{k_0+1}$,
- for the other $J_{\tilde{\boldsymbol{\beta}}}$ many j's, we have $E^{k_0+r-s}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) < e_0^{\boldsymbol{l}^{(j)}}(\tilde{\boldsymbol{\theta}} + t\tilde{\boldsymbol{\beta}}) < 0 = \min F_0^{k_0}$.

Hence

$$J_{\tilde{\boldsymbol{\beta}}} = r - s - 1. \tag{5.18}$$

Thus combining (5.17) with (5.18), we have

$$2s - r = J_0 - 2. \tag{5.19}$$

This contradicts (5.14) since $J_{\boldsymbol{\beta}}^0 \geq 1$. □

6. Example with exactly two intervals

Let all the q_i's be even and $\delta > 0$ be any small positive number. We are going to construct V with minimal period $\boldsymbol{q}$, such that $\|V\|_\infty = \delta$ and the spectrum of H_V does not contain the point 0. This example is a modification of Krüger's example (see Theorem 6.3 in [5]), where V is $(2, 2, ..., 2)$-periodic.

Let us define

$$V_{\boldsymbol{q}}(\boldsymbol{n}) = \begin{cases} (1 - \delta^2/d)\delta & \text{if } \boldsymbol{n} \equiv \mathbf{0} \pmod{\boldsymbol{q}} \\ \delta(-1)^{|\boldsymbol{n}|} & \text{otherwise} \end{cases} \tag{6.1}$$

It can be easily checked that $V_{\boldsymbol{q}}$ has minimal period $\boldsymbol{q}$ and $\|V\|_\infty = \delta$. The fact that the spectrum of H_V does not contain 0 will follow from the following lemma.

Lemma 6.1. *There exists constant $\delta_0 > 0$ such that for any $0 < \delta < \delta_0$, we have*

$$\|(H_0 + V_{\boldsymbol{q}})u\| > \frac{1}{2}\delta$$

holds for any unit vector $u \in l^2(\mathbb{Z}^d)$.

Proof of Lemma 6.1. Let us consider

$$\|(H_0+V_{\boldsymbol{q}})u\|^2=\|H_0u\|^2+\|V_{\boldsymbol{q}}u\|^2+2(H_0u,V_{\boldsymbol{q}}u)\geq\|V_{\boldsymbol{q}}u\|^2+2(H_0u,V_{\boldsymbol{q}}u), \tag{6.2}$$

in which the first term obviously satisfies

$$\|V_{\boldsymbol{q}}u\|^2=\sum_{\boldsymbol{n}\in\mathbb{Z}^d}|V_{\boldsymbol{q}}(\boldsymbol{n})|^2|u(\boldsymbol{n})|^2\geq(1-\delta^2/d)^2\delta^2\geq(1-\delta^2)^2\delta^2. \tag{6.3}$$

Let $\{\boldsymbol{b}_i\}$ be the standard basis for $\mathbb{R}^d$. The second term in (6.2) could be estimated in the following way:

$$\begin{aligned}(H_0u,V_{\boldsymbol{q}}u)&=\sum_{\boldsymbol{n}\in\mathbb{Z}^d}\left(\sum_{i=1}^d u(\boldsymbol{n}\pm\boldsymbol{b}_i)\right)V_{\boldsymbol{q}}(\boldsymbol{n})u(\boldsymbol{n})\\ &=\sum_{i=1}^d\sum_{\boldsymbol{n}\in\mathbb{Z}^d}u(\boldsymbol{n}+\boldsymbol{b}_i)u(\boldsymbol{n})(V_{\boldsymbol{q}}(\boldsymbol{n})+V_{\boldsymbol{q}}(\boldsymbol{n}+\boldsymbol{b}_i)).\end{aligned} \tag{6.4}$$

Note that by our construction and the fact that q_i's are even,

$$V_{\boldsymbol{q}}(\boldsymbol{n})+V_{\boldsymbol{q}}(\boldsymbol{n}+\boldsymbol{b}_i)=\begin{cases}-\delta^3/d & \text{if } \boldsymbol{n}\equiv-\boldsymbol{b}_i \text{ or } \boldsymbol{0} \pmod{\boldsymbol{q}}\\ 0 & \text{otherwise}\end{cases} \tag{6.5}$$

Combining (6.4) with (6.5), we get

$$|(H_0u,V_{\boldsymbol{q}}u)|\leq\frac{\delta^3}{d}\sum_{i=1}^d\sum_{\boldsymbol{n}\in\mathbb{Z}^d}|u(\boldsymbol{n}+\boldsymbol{b}_i)||u(\boldsymbol{n})|\leq\delta^3. \tag{6.6}$$

Now combining (6.2), (6.3) with (6.6), we get

$$\|(H_0+V_{\boldsymbol{q}})u\|^2\geq(1-\delta^2)^2\delta^2-2\delta^3>\frac{1}{4}\delta^2,$$

provided δ small. □

Appendix A.

Proof of Lemma 4.1. Without loss of generality we could assume $E\geq 0$.

If $d=2\tilde{d}$ is an even number, then we could take $(0,1/2)\ni\theta_1=\cdots=\theta_{\tilde{d}}=1-\theta_{\tilde{d}+1}=\cdots=1-\theta_{2\tilde{d}}$ be such that $\cos 2\pi\theta_1=\frac{E}{4\tilde{d}}\neq\pm 1$.

If $d=2\tilde{d}+1$ is an odd number and $E\in[2,4\tilde{d}+2)$, then we could take $\theta_{2\tilde{d}+1}=0$ and $(0,1/2)\ni\theta_1=\cdots=\theta_{\tilde{d}}=1-\theta_{\tilde{d}+1}=\cdots=1-\theta_{2\tilde{d}}$ be such that $\cos 2\pi\theta_1=\frac{E-2}{4\tilde{d}}\neq\pm 1$.

If $d=2\tilde{d}+1$ is an odd number and $E\in[0,2)$, then we could take $\theta_{2\tilde{d}+1}=\frac{1}{2}$ and $(0,1/2)\ni\theta_1=\cdots=\theta_{\tilde{d}}=1-\theta_{\tilde{d}+1}=\cdots=1-\theta_{2\tilde{d}}$ be such that $\cos 2\pi\theta_1=\frac{E+2}{4\tilde{d}}\neq\pm 1$. □

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