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Lattice Points, Perturbation Theory and the Periodic Polyharmonic Operator

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1 Introduction

Consider the polyharmonic operator acting in $L^2(\mathbb{R}^d)$, perturbed by a real-valued periodic function:

$$H = H_0 + V,\ H_0 = (-\Delta)^l, \quad l > 0. \tag{1.1}$$

The spectrum of H is formed from closed intervals (*spectral bands*), possibly separated by *gaps* (see [6], [10]). We shall concentrate on one aspect of this structure, known as the Bethe-Sommerfeld conjecture, which states that the *number of spectral gaps is finite*. This hypothesis was put forward by H. Bethe and A. Sommerfeld for the Schrödinger operator in dimension three, i.e. for $l = 1, d = 3$. Ever since, the case $l = 1$ was a subject of intensive study by a number of authors, which lead to the justification of the conjecture for $d = 2$ in [9], [1], for $d = 3$ in [13] and for $d = 2, 3, 4$ in [2]. In dimensions $d \geq 5$ the problem was solved only for rational lattices of periods (see [12]). For arbitrary l the number of gaps was shown to be finite for $2l > d, d \geq 3$ in [11], [12]. Later, in [3] (see also [4]), these conditions were relaxed to $4l > d + 1,\ d \geq 2$. In our recent paper [7] we prove the conjecture for $6l > d + 2, d \geq 2$.

The aim of the present paper is to loosen the condition from [7] further. Namely, we show that the number of gaps in the spectrum of H is finite if $8l > d+3$, $d \geq 2$. In the physically most relevant case $l = 1$ (i.e. for the Schrödinger operator), this requirement is fulfilled for $d = 2, 3$ or 4. These are exactly the dimensions for which the conjecture was justified in the papers cited above. However, our method has a considerable advantage that it relies only on elementary perturbation theoretic arguments and treats all dimensions d and exponents l satisfying $8l > d + 3$, in a unified fashion. In connection with this, it is appropriate to note that the study of the polyharmonic operator with an arbitrary $l > 0$ (rather than with $l = 1$ only) is useful and instructive as it allows one to understand better the mechanisms responsible for the quantitative characteristics of the spectrum, and to find out how far one can push the perturbation theoretic argument in its investigation.

Our approach follows the plan of [7] and comprises two main ingredients:

1. Number-theoretic estimates, more precisely, estimates on the number of lattice points inside a ball of a large radius;

2. An estimate on the difference between the counting functions of the perturbed and unperturbed problems.

All the necessary number-theoretic facts were obtained in the previous article [7] and are used here without any modifications (see Proposition 3.1). On the contrary, for ingredient 2 we now rely on a bound (see Proposition 3.2), borrowed from [5], which is more precise than the corresponding bound established in [7]. This modification enabled us to improve the sufficient condition of validity of the Bethe-Sommerfeld conjecture from $6l > d+2$ to $8l > d+3$. Before we learnt about the existence of paper [5] we established an alternative version of Proposition 3.2, which required the condition $V \in \mathsf{C}^\infty$, which is more restrictive in comparison with [5]. This version can be found in [8].

Notation. By bold lowercase letters we denote vectors in $\mathbb{R}^d$ and $\mathbb{Z}^d$, e.g. $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{m} \in \mathbb{Z}^d$. Bold uppercase letters $\mathbf{G}, \mathbf{F}$ are used for $d \times d$ constant positive definite matrices. The notations $\mathbf{ab}$ and $\mathbf{aGb}$ stand for the scalar product in $\mathbb{R}^d$ and the bilinear form of the matrix $\mathbf{G}$ respectively. For any function $f \in L^1(\mathcal{O})$, $\mathcal{O} = [0, 2\pi)^d$ the Fourier transform is defined as follows:

$$\hat{f}(\mathbf{m}) = \frac{1}{(2\pi)^{d/2}} \int_{\mathcal{O}} e^{-i\mathbf{mx}} f(\mathbf{x}) d\mathbf{x}.$$

Throughout the paper we also use the following notation:

$$\delta = \delta_d = \begin{cases} 0, & d \neq 1 (\operatorname{mod} 4); \\ \text{arbitrary positive number}, & d = 1 (\operatorname{mod} 4). \end{cases} \tag{1.2}$$

By C and c (with or without indices) we denote various positive constants whose precise value is unimportant.

2 Main result and preliminaries

2.1 Notation and main result

Using a linear change of coordinates, (1.1) can be transformed to the following form:

$$\begin{aligned} H =& H_0 + V, \\ H_0 =& H_0^{(l)} = (\mathbf{DGD})^l, \ \mathbf{D} = -i\nabla, \end{aligned}$$

where $\mathbf{G}$ is a constant positive-definite $d \times d$ -matrix, and V is a bounded real-valued function periodic with respect to the cubic lattice $\Gamma = (2\pi\mathbb{Z})^d$. As V is bounded, the operator H is self-adjoint on the domain $D(H_0) = H^{2l}(\mathbb{R}^d)$. We use the following notation for the fundamental domains of the lattice Γ and its dual lattice $\Gamma^\dagger = \mathbb{Z}^d$:

$$\mathcal{O} = [0, 2\pi)^d, \ \mathcal{O}^\dagger = [0, 1)^d.$$

Let us also introduce the torus $\mathbb{T}^d = \mathbb{R}^d/\Gamma$. To describe the spectrum of H we use the Floquet decomposition of the operator H (see [10]). We identify the space $L^2(\mathbb{R}^d)$ with the direct integral

$$\mathfrak{G} = \int_{\mathcal{O}^\dagger} \mathfrak{H} d\mathbf{k}, \ \mathfrak{H} = L^2(\mathcal{O}).$$

The identification is implemented by the Gelfand transform

$$(Uu)(\mathbf{x}, \mathbf{k}) = e^{-i\mathbf{kx}} \sum_{\mathbf{m}\in\mathbb{Z}^d} e^{-i2\pi\mathbf{km}} u(\mathbf{x} + 2\pi\mathbf{m}), \ \mathbf{k} \in \mathbb{R}^d,$$

which is initially defined on functions from the Schwarz class and extends by continuity to a unitary mapping from $L^2(\mathbb{R}^d)$ onto $\mathfrak{G}$. It is readily seen that

$$(UH_0U^{-1}u)(\ \cdot\ , \mathbf{k}) = H_0(\mathbf{k})u(\ \cdot\ , \mathbf{k}),$$
$$H_0(\mathbf{k}) = \big((\mathbf{D} + \mathbf{k})\mathbf{G}(\mathbf{D} + \mathbf{k})\big)^l, \ \mathbf{k} \in \mathbb{R}^d,$$

with the domain $D(H_0(\mathbf{k})) = H^{2l}(\mathbb{T}^d)$. The family $H(\mathbf{k}) = H_0(\mathbf{k}) + B(\mathbf{k})$ realises the decomposition of H in the direct integral:

$$UHU^{-1} = \int_{\mathcal{O}^\dagger} H(\mathbf{k}) d\mathbf{k}.$$

The spectra of all $H(\mathbf{k})$ consist of discrete eigenvalues $\lambda_j(\mathbf{k}), j = 1, 2, \dots,$ that we arrange in non-decreasing order counting multiplicity. It is clear that $\lambda_j(\ \cdot\ )$ are continuous functions of $\mathbf{k}$. The images

$$\ell_j = \cup_{\mathbf{k}\in\overline{\mathcal{O}^\dagger}} \lambda_j(\mathbf{k}),$$

of the functions λ_j are called *spectral bands*. The spectrum of the initial operator H has the following representation:

$$\sigma(H) = \cup_j \ell_j.$$

The bands with distinct numbers may overlap. To characterise this overlapping we introduce the function $\mathfrak{m}(\lambda) = \mathfrak{m}(\lambda, V)$ called *the multiplicity of overlapping*, which is equal to the number of bands containing given point $\lambda \in \mathbb{R}$:

$$\mathfrak{m}(\lambda) = \#\{j : \lambda \in \ell_j\};$$

and the *overlapping function* $\zeta(\lambda) = \zeta(\lambda, V), \ \lambda \in \mathbb{R}$, defined as the maximal number t such that the symmetric interval $[\lambda - t, \lambda + t]$ is entirely contained in one of the bands ℓ_j:

$$\zeta(\lambda) = \max_j \max\{t : [\lambda - t, \lambda + t] \subset \ell_j\}.$$

These two quantities were first introduced by M. Skriganov (see e.g. [12]). It is easy to see that ζ is a continuous function of $\lambda \in \mathbb{R}$.

To state the main result we have to impose additional smoothness conditions on the potential V. It will be convenient to formulate them in terms of the Fourier coefficients $\hat{V}(\boldsymbol{\theta})$ of the potential V. We shall assume that

$$\sum_{\boldsymbol{\theta} \in \mathbb{Z}^d} |\hat{V}(\boldsymbol{\theta})| \, |\boldsymbol{\theta}|^{\nu} < \infty, \tag{2.1}$$

with

$$\nu > \begin{cases} (d-1)/2, \ d \geq 3; \\ 2(l+1)/3, \ d = 2. \end{cases} \tag{2.2}$$

This condition is exactly the same as in Section 1 of [5]. The main results of the paper are stated in the following theorem. Recall that the parameter $\delta = \delta_d$ used in the Theorem is defined in (1.2).

Theorem 2.1. *Let $l > 0$, $d \geq 2$ and let $V \in C^{\infty}(\mathbb{T}^d)$ be a real-valued function satisfying the conditions* (2.1), (2.2). *Suppose that $8l > d + 3$. Then there is a number $\lambda_{\mathrm{l}} = \lambda_{\mathrm{l}}(V, \delta) \in \mathbb{R}$ such that*

$$\mathfrak{m}(\lambda) \geq c_0 \lambda^{\frac{d-1}{4l} - \delta}, \quad \zeta(\lambda) \geq c_0 \lambda^{1 - \frac{d+1}{4l} - \delta} \tag{2.3}$$

for all $\lambda \geq \lambda_{\mathrm{l}}$ with a constant c_0 independent of V.

Clearly, this Theorem implies the validity of the Bethe-Sommerfeld conjecture.

The proof of Theorem 2.1 exploits the connection between the functions $\mathfrak{m}(\lambda), \zeta(\lambda)$ and the counting functions

$$N\big(\lambda; H(\mathbf{k})\big) = \sum_{\lambda_j(\mathbf{k}) \leq \lambda} 1, \quad n\big(\lambda; H(\mathbf{k})\big) = \sum_{\lambda_j(\mathbf{k}) < \lambda} 1.$$

Denote

$$N_+(\lambda) = \max_{\mathbf{k}} N\big(\lambda; H(\mathbf{k})\big), \ N_-(\lambda) = \min_{\mathbf{k}} N\big(\lambda; H(\mathbf{k})\big),$$

and similarly define $n_{\pm}(\lambda)$. It is easy to deduce from the definitions of $\mathfrak{m}(\lambda), \zeta(\lambda)$ (see e.g. [12], [13]) that

$$\begin{gathered} \mathfrak{m}(\lambda) = N_+(\lambda) - n_-(\lambda), \\ \zeta(\lambda) = \sup\{t : N_-(\lambda + t) < N_+(\lambda - t)\}, \end{gathered} \tag{2.4}$$

which immediately implies that

$$\mathfrak{m}(\lambda) \geq N_+(\lambda) - N_-(\lambda). \tag{2.5}$$

The proof of Theorem 2.1 is completed in the next section.

3 Proof of the main theorem

We begin with a description of two key ingredients of the proof of Theorem 2.1.

3.1 Integer points in the ellipsoid

In this subsection we collect some facts from number theory that will play a crucial role.

Let $\mathcal{C} \subset \mathbb{R}^d$ be a measurable set and let $\mathcal{C}^{(\mathbf{k})}$, $\mathbf{k} \in \mathcal{O}^\dagger$ be the family of sets obtained by shifting $\mathcal{C}$ by the vector $-\mathbf{k}$, i.e.

$$\mathcal{C}^{(\mathbf{k})} = \{\boldsymbol{\xi} \in \mathbb{R}^d : \boldsymbol{\xi} + \mathbf{k} \in \mathcal{C}\}.$$

The characteristic function of the set $\mathcal{C}$ will be denoted by $\chi(\,\cdot\,;\mathcal{C})$. Denote by $\#(\mathbf{k};\mathcal{C})$ the number of integer points in $\mathcal{C}^{(\mathbf{k})}$, i.e.

$$\#(\mathbf{k};\mathcal{C}) = \sum_{\mathbf{m}\in\mathbb{Z}^d} \chi(\mathbf{m}+\mathbf{k};\mathcal{C}).$$

Introduce the notation

$$\langle f\rangle = \int_{\mathcal{O}^\dagger} f(\mathbf{k})d\mathbf{k}$$

for the average value of a function $f \in L^1(\mathcal{O}^\dagger)$. Then the previous formula immediately leads to the equality

$$\langle \#(\mathcal{C})\rangle = \mathrm{vol}(\mathcal{C}).$$

We shall need an estimate for the number of integer points inside an (closed) ellipsoid determined by the matrix $\mathbf{G}$. Precisely, for any $\rho > 0$ let $\mathcal{E}(\rho) = \mathcal{E}(\rho, \mathbf{F}) \subset \mathbb{R}^d$ be the ellipsoid

$$\{\boldsymbol{\xi} \in \mathbb{R}^d : |\mathbf{F}\boldsymbol{\xi}| \le \rho\},\ \ \mathbf{F} = \mathbf{G}^{1/2}.$$

There is a very simple connection between integer points in the ellipsoid and the eigenvalues of the unperturbed problem. Indeed, the eigenvalues of the operator $H_0(\mathbf{k})$ equal $|\mathbf{F}(\mathbf{m}+\mathbf{k})|^{2l}$, $\mathbf{m} \in \mathbb{Z}^d$, which ensures that for all $\rho \ge 0$

$$\begin{cases} N\big(\rho^{2l}; H_0(\mathbf{k})\big) = \#\big(\mathbf{k}; \mathcal{E}(\rho)\big), \\ \big\langle N(\rho^{2l}; H_0)\big\rangle = \big\langle \#(\mathcal{E}(\rho))\big\rangle = \mathrm{w}_d\,\rho^d, \end{cases} \tag{3.1}$$

where

$$\mathrm{w}_d = \frac{K_d}{\sqrt{\det \mathbf{G}}},\quad K_d = \frac{\pi^{d/2}}{\Gamma(d/2+1)},$$

K_d being the volume of the unit ball in $\mathbb{R}^d$. We are interested in the lower bound for the deviation of the function $N(\rho^{2l}; H_0(\mathbf{k}))$ from the volume $\mathrm{w}_d\,\rho^d$ of the ellipsoid $\mathcal{E}(\rho)$ as $\rho \to \infty$:

Proposition 3.1. *Let the number δ be as defined in* (1.2). *Then for all sufficiently big ρ the estimate holds:*

$$\big\langle \big|\#\big(\mathcal{E}(\rho)\big) - \mathrm{w}_d\, \rho^d\big|\big\rangle \ge C\rho^{\frac{d-1}{2}-\delta},$$

with a constant $C = C(d, \mathbf{G}, \delta)$.

Note that we do not need any upper bound on the l.h.s. of the above inequality. We refer to [7] for the proof and discussion of Proposition 3.1.

3.2 An estimate for the counting function $N(\rho^{2l}; H(\mathbf{k}))$

As in [7], the second crucial ingredient of the proof is an estimate for the deviation of $N(\lambda; H(\mathbf{k}))$ from the unperturbed counting function $N(\lambda; H_0(\mathbf{k}))$, *averaged* in $\mathbf{k} \in \mathcal{O}^\dagger$. In contrast to [7], we use a more precise estimate established in [5]:

Proposition 3.2. *Let $d \ge 2$, $2l > 1$. Suppose that the potential satisfies the conditions* (2.1), (2.2). *Then*

$$\big\langle \big|N(\rho^{2l}; H) - N(\rho^{2l}; H_0)\big|\big\rangle \le C\rho^{d+1-4l} \ln \rho, \tag{3.2}$$

for sufficiently large ρ.

The bound (3.2) was derived in [5] as an intermediate result for obtaining the corresponding estimate for the *integrated density of states* $D(\rho^{2l}; H) = \langle N(\rho^{2l}; H)\rangle$. Indeed, by (3.1), the unperturbed density of states $D(\rho^{2l}; H_0)$ coincides with $\mathrm{w}_d\, \rho^d$, so that (3.2) leads to

$$D(\rho^{2l}; H) = \mathrm{w}_d\, \rho^d + \rho^{d+1-4l} O\big(\ln \rho\big),\ \ \rho \to \infty.$$

For $l = 1$ and $V \in \mathsf{C}^\infty(\mathbb{T}^d)$ a similar estimate with the remainder $O(\rho^{d-3+\eta})$ with arbitrary $\eta > 0$ was proved in [2] for all $d \ge 2$.

Note also that for $V \in \mathsf{C}^\infty(\mathbb{T}^d)$ and arbitrary $l > 1/2$ an estimate similar to (3.2) with the remainder $O(\rho^{d+1-4l+\eta})$ with arbitrary $\eta > 0$ was found in [8].

3.3 Proof of Theorem 2.1

Observe that under the condition $8l > d + 3$ we have $d + 1 - 4l < (d - 1)/2$. Therefore Proposition 3.2 and (3.1) give the equalities

$$\lim \rho^{-\beta} \langle \big|N(\rho^{2l}; H) - N(\rho^{2l}; H_0)\big|\rangle = 0, \tag{3.3}$$

$$\lim \rho^{-\beta} \big|\langle N(\rho^{2l}; H)\rangle - \mathrm{w}_d\, \rho^d\big| = 0, \tag{3.4}$$

as $\rho \to \infty$, for $\beta = (d - 1)/2 - \delta$ with a sufficiently small δ (see (1.2) for definition of δ). Note that

$$\begin{aligned} \big\langle |N(\lambda; H) - \langle N(\lambda; H)\rangle|\big\rangle \ge{}& \big\langle |N(\lambda; H_0) - \mathrm{w}_d\, \rho^d|\big\rangle \\ &- \big\langle |N(\lambda; H) - N(\lambda; H_0)|\big\rangle \\ &- |\langle N(\lambda; H)\rangle - \mathrm{w}_d\, \rho^d|,\ \ \lambda = \rho^{2l}. \end{aligned}$$

Now, using Proposition 3.1 and (3.1) for the first term in the r.h.s., and the relations (3.3) and (3.4) for the remaining terms, we obtain that

$$\left\langle \left| N(\rho^{2l}; H) - \langle N(\rho^{2l}; H)\rangle \right| \right\rangle \geq c\rho^{\beta},$$

for all $\rho \geq \rho_0$ with a sufficiently large $\rho_0 > 0$. Noticing that the function in the l.h.s. is of average zero, we see that

$$\max_{\mathbf{k}} N\big(\rho^{2l}; H(\mathbf{k})\big) \geq \langle N(\rho^{2l}; H)\rangle + c\rho^{\beta},$$

$$\min_{\mathbf{k}} N\big(\rho^{2l}; H(\mathbf{k})\big) \leq \langle N(\rho^{2l}; H)\rangle - c\rho^{\beta},$$

which implies, in view of (3.4), that

$$\begin{cases} \max_{\mathbf{k}} N\big(\rho^{2l}; H(\mathbf{k})\big) \geq & \mathrm{w}_d\, \rho^d + c\rho^{\beta}, \\ \min_{\mathbf{k}} N\big(\rho^{2l}; H(\mathbf{k})\big) \leq & \mathrm{w}_d\, \rho^d - c\rho^{\beta}, \end{cases} \tag{3.5}$$

for $\rho \geq \rho_0$. According to (3.5) for all non-negative $t \leq \rho^{2l}/2$ we have

$$\begin{aligned} N_+(\rho^{2l} - t) \geq &\ \mathrm{w}_d(\rho^{2l} - t)^{\frac{d}{2l}} + C(\rho^{2l} - t)^{\frac{\beta}{2l}} \\ \geq &\ \mathrm{w}_d\, \rho^d + C\rho^{\beta} - ct\rho^{d-2l}, \quad \forall \rho \geq 2\rho_0. \end{aligned}$$

Similarly,

$$\begin{aligned} N_-(\rho^{2l} + t) \leq &\ \mathrm{w}_d(\rho^{2l} + t)^{\frac{d}{2l}} - C(\rho^{2l} + t)^{\frac{d}{2l}} \\ \leq &\ \mathrm{w}_d\, \rho^d - C\rho^{\beta} + ct\rho^{d-2l}, \quad \forall \rho \geq \rho_0. \end{aligned}$$

Now one concludes from (2.5) that

$$\mathfrak{m}(\rho^{2l}) \geq N_+(\rho^{2l}) - N_-(\rho^{2l}) \geq 2C\rho^{\beta}, \ \forall \rho \geq 2\rho_0,$$

and hence

$$\mathfrak{m}(\lambda) \geq c\lambda^{\frac{\beta}{2l}},$$

which yields (2.3) for all $\lambda \geq \lambda_{\mathrm{l}} = (2\rho_0)^{2l}$. This completes the proof of the lower bound for $\mathfrak{m}(\lambda)$. To estimate $\zeta(\lambda)$ write

$$N_+(\rho^{2l} - t) - N_-(\rho^{2l} + t) \geq 2C\rho^{\beta} - 2ct\rho^{d-2l}.$$

From the formula (2.4) one can now infer (2.3) for $\zeta(\lambda), \lambda \geq (2\rho_0)^{2l}$.

Theorem 2.1 is proved. $\square$

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