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Eigenvalues and Dislocation of Lattice

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Abstract

Can one hear the shape of a drum? It proposed by Kac in 1966. The simple answer is NO as shown through the construction of iso-spectral domains. However, the method and the idea to detect the shape of the domain can be applied to many fields. In this paper, we give an analytic method to detect the dislocation of the lattice. Moreover, if the dislocation became the acute trapezoid, we give a method to distinguish the shape by getting the eigenvalue.

格子の固有値と 転位

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概要

太鼓の形が聞こえますか. それは 1966 年に Kac によって提案されました. 簡単な答えは等スペクト ル領域の構築を 通して示されるように NO です. しかしながら, ドメインの形状を 検出する 方法およびアイデアは, 多くの分野に適用することができる. 本論文では, 格子の転位を 検出するための解析法を 与える. さらに, 転位が鋭い梯形になった場合, 固有値を 求めることで形状を 区別する 方法を 示します.

1 Introduction

In crystallography, crystal structure is a description of the ordered arrangement of atoms, ions or molecules in a crystalline material [3]. Ordered structures occur from the intrinsic nature of the constituent particles to form symmetric patterns that repeat along the principal directions of three-dimensional space in matter. The dislocation of lattice is one of popular tops in studying the lattice, in this paper we focus on the two-dimensional lattice and show how to detect the dislocation by analysis techniques. The theory describing the elastic fields of the defects was originally developed by Volterra [9]. The term 'dislocation' referring to a defect on the atomic scale, which was coined by Taylor [8]. Some types of dislocations can be visualized as being caused by the termination of a plane of atoms in the middle of a crystal. In such a case, the surrounding planes are not straight, however they bend around the edge of the terminating plane so that the crystal structure is perfectly ordered on either side. This phenomenon is analogous to the following situation related to a stack of paper: If half of a piece of paper is inserted into a stack of paper, the defect in the stack is noticeable only at the edge of the half sheet. In this paper, we give an analytic method to detect the dislocation and categorize the dislocation into some cases. From Oct. 2017 to Oct. 2018, the author joined the program of Mathematical science practice research(数理科学実践研究) at Graduate School of Mathematical Sciences, The University of Tokyo. During the practice, the author found the relation between eigenvalues and dislocation. The purpose of this paper is to understand the dislocation from the viewpoint of the eigenvalue or equation.

In this paper, we focus on 2-dimensional crystallography. First, we give a brief introduction to the Kac problem in mathematical viewpoint to the readers who are not so familiar with. On the plane $\mathbb{R}^2$, given a bounded region Ω. If one makes drum with exactly the same shape of Ω, then we can hear the rhythms of the drum. Weyl [10] discovered the first geometric spectral invariant: If two drums sound the same, then they have the same area. Kac [6] posed a question: whether or not the drum must have the same shape? The methods used to understand this problem draw on diverse areas: e.g. partial differential equations, dynamical systems, group theory, number theory and probability.

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We translate the problem into mathematical language as following: Suppose that we know all the eigenvalues $0 < \lambda_1 < \lambda_2 < \cdots \to \infty$ of a bounded region Ω, i.e. each λ_i solves the equation

$$\begin{cases} -\Delta u = \lambda_i u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \tag{1}$$

where $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. Then, can we determine the shape of Ω uniquely?
For example, in 1-dimensional case, as for any connected bounded set Ω of $\mathbb{R}$ is an interval with length l. Without loss of generality, we assume $\Omega = [0, l]$.

$$\begin{cases} -\Delta u = \lambda u & (0, l), \\ u = 0 & \{0, l\}. \end{cases} \tag{2}$$

We know $\lambda_n = (n\pi/l)^2$, $u_n(t) = \sin(\frac{n\pi}{l} t)$. Thus, if we get all the eigenvalues, we know the length of this region, i.e. it is uniquely determined. However, the answer is **NO** in 2-dimensional case. The example was given by Carol Gordon, David Webb, and Scott Wolpert [5]. The following pictures show that even though they are different, their corresponding eigenvalues are exactly the same.

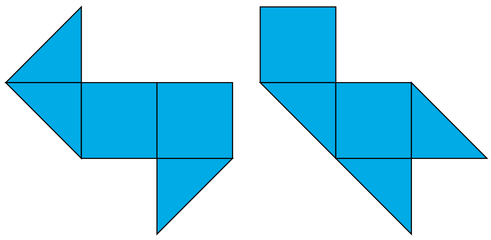

Figure 1: different shapes with the same eigenvalues

In this paper, we introduce an analytic method to distinguish the shape of some special trapezoid. For a two-dimensional lattice, by hearing the spectrum, we know the the shape, i.e. width and height of each unit. To distinguish the shapes of the dislocation, we need some assumptions:

Assumption 1 *We assume that the standard crystallography is a rectangle. Moreover, we assume that dislocation becomes a trapezoid.*

Under the above Assumption 1, we can distinguish the dislocations by the following Theorem.

Theorem 2 *Let Ω be a bounded in region of $\mathbb{R}^2$. Suppose that we know all the eigenvalues $0 < \lambda_1 < \lambda_2 < \cdots \to \infty$, of Laplacian operator with Dirichlet boundary on $\partial\Omega$,i.e. each λ_i solves the following equation*

$$\begin{cases} -\Delta u = \lambda_i u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases} \tag{3}$$

If Ω is either acute trapezoid, isosceles trapezoid or right trapezoid, then the exact shape of Ω can be uniquely determined.

The organization of the paper is the following: in Section 2, we give a preliminary to the heat kernel and asymptotic formula about the trace of the heat kernel, asymptotic formula about the trace of the heat kernel and the sketch proof of Theorem 2.

2 History and sketch proof of Theorem 2

Firstly, we recall the heat kernel of the Euclidean space. The heat kernel in $\mathbb{R}^2$ is given by

$$H(p,q,t) = \frac{1}{4\pi t} \exp\left(-\frac{dist^2(p,q)}{4t}\right),$$

where $dist(p,q)$ denotes the Euclidean distance between the two points p and q. If we take a trace, we have

$$\sum_{i=1}^{\infty} e^{-\lambda_i t} = Tr(H(p,q;t)) =: H(t).$$

By Weyl [1, Chapert 1], we know that

$$H(t) \sim \frac{A}{4\pi t} - \frac{P}{8\sqrt{\pi t}} + O(1),$$

where A denotes the area of Ω and P denotes the perimeter of $\partial\Omega$. On polygon , Grieser and Maronna [4] gave an asymptotic formula,

$$H(t) \sim \frac{A}{4\pi t} - \frac{P}{8\sqrt{\pi t}} + \frac{1}{24}(\sum_{i=1}^{n} \frac{\pi}{\theta_i} - \frac{\theta_i}{\pi}), \tag{4}$$

where θ_i denotes the interior angles. Therefore, we have the following theorem.

Theorem 3 (Grieser and Maronna) *Let Ω be a triangle of the 2-dimensional Euclid space $\mathbb{R}^2$. Suppose that the eigenvalues of the Laplacian operator with Dirichlet boundary condition are known. Then we can determinate the shape of Ω.*

Proof For any triangle, let A denote its area, P denote its perimeter and θ_i denote the three angles for $i = 1, 2, 3$. The idea is straightforward. Since any triangle is uniquely determined by

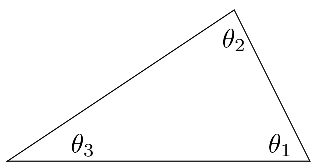

Figure 2: triangle

- its area A,
- $A/P^2 = \cot(\theta_1/2) + \cot(\theta_2/2) + \cot(\theta_3/2)$,
- $\frac{1}{\theta_1} + \frac{1}{\theta_2} + \frac{1}{\theta_2}$.

Together with the formula 4, we have our desired result. □

However to determinate a trapezoid or a convex quadrilateral, the above conditions are not sufficient. On the other hand, Duistermaat and Guillemin [2] showed that the singularities of the wave trace

$$\sum_{i=1}^{\infty} e^{i\sqrt{\lambda_i}t} =: W(t),$$

are contained in the length spectrum, i.e. $h \in Sing(W(t))$.
Now we give the proof of our main theorem.
Proof(of Theorem 2) We divide the proof into three cases and begin from the easiest case.
(1) Isosceles trapezoid.

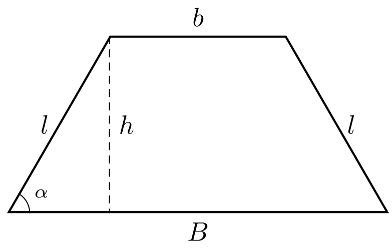

Figure 3: isosceles trapezoid

By the similar argument of Theorem 3, we have that: If Ω is an isosceles trapezoid and we get the eigenvalues

$$\lambda_1 < \lambda_2, \cdots,$$

of the equation (3), then we know the height h, Perimeter P, and area A. Let l denote the length of a leg. By the straightforward calculation, we have that

$$A = \frac{1}{2}(b+B)h,\ h/\sin\alpha = l.$$

Under the hypothesis, one gets

$$l = \frac{1}{2}(P - 2A/h),\ \alpha = \sin^{-1}(\frac{2h}{P - \frac{2A}{h}}),$$

which implies that the shape of isosceles trapezoid is uniquely determined.

(2) Right trapezoid. Since one angle is known $\frac{\pi}{2}$, we can apply the methods to determine the

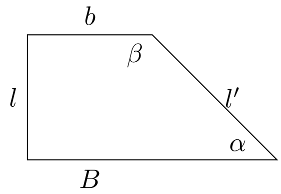

Figure 4: right trapezoid

shape, here we omit the proof.
(3) For the acute trapezoid, i.e. the sum of the bottom angles is less than $\frac{\pi}{2}$.

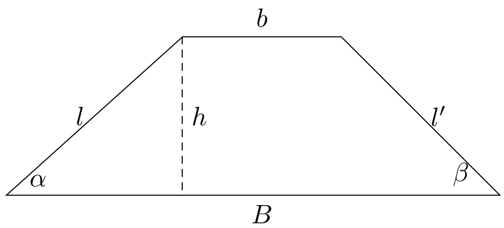

Figure 5: acute trapezoid

Clearly, given the eigenvalues, we have the the following four identities:

$$l = \frac{h}{\sin\alpha},\ l' = \frac{h}{\sin\beta},$$

$$B + b = \frac{2A}{h},\ l + l' = P - (B + b).$$

Therefore, it suffices to determine α and β. The following lemma provides us an answer to determining the bottom angles. □

Lemma 4 (Lu and Rowlett [7]) *Let $p, q \in \mathbb{R}$ satisfy*

$$\begin{cases} \csc\alpha + \csc\beta = p, \\ \frac{1}{\alpha(\pi-\alpha)} + \frac{1}{\alpha(\pi-\alpha)} = q. \end{cases} \tag{5}$$

If $0 < \beta \leq \alpha < \frac{\pi}{2}$, for any p and q satisfy the above equation, then there exists a unique solution (α, β).

So far, we have shown our main theorem. But for the other cases, e.g. random trapezoid, it is not clear whether the eigenvalues can determine the shape or not.

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