Hearing the Symmetries of Crystal Lattices from the Integrated Acoustic Spectrum

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Abstract

Let $C$ be a crystal and $\phi$ be a periodic realization of it in $\mathbb{R}^n$, also let $L$ be the lattice group of $\phi(C)$ which preserves the covering space nature of crystal lattices. In this article, firstly, we define the concept of acoustic spectrum of the crystal lattice $C$ and then provide the algebraic formalism of the question of finding the frequencies of the torus $\mathbb{R}^n/L$, when the set of acoustic spectrum is known. An answer for crystals with uniform atomic force constants is given.

Keywords: Crystal lattice, Character group, Acoustic phase velocity, Elastic Laplacian Operator.

1. Introduction

Laplace-Beltrami operator is a natural second order elliptic operator on a Riemannian manifold defined as $\text{div} \circ \text{grad}$. It is well known that on a closed manifold, this operator has discrete positive eigenvalues with finite multiplicities [4]. Two Riemannian manifolds are isospectral if their Laplace-Beltrami operator have the same spectrum, considering multiplicities. A fundamental question by Mark Kac asks whether it is possible to find two nonisometric isospectral manifolds. The first answer to this question was provided by Milnor’s 16 dimensional tori that is a geometric realization of self-dual lattices with the same theta functions [3]. Naturally, lattices appear in the theory of crystallography as symmetries of a crystal lattice. We mean by a crystal lattice, a periodic harmonic realization of a commutative covering space of a finite graph. In the nature, the interatomic forces lead to oscillations of crystal’s atoms around their equilibrium positions. These oscillations are called crystal lattice vibrations. Physicists usually decompose the system of oscillations into independent simple harmonic oscillators, and calculate the distribution of vibration frequencies [4]. This method is the same as the theory
of Fourier series for a vibrated chord. Acoustic phase velocities are the phase velocity of elastic waves in the uniform elastic body corresponding to the crystal lattice. In this article we consider the integration of acoustic phase velocity in the direction of closed geodesics of the lattice character group and we find the algebraic formalism of hearing the eigenvalues of Laplacian (or equivalently the frequencies) on the torus \( \mathbb{R}^n/L \).

This paper is organized as follows. In section 2 a review of the notion of a crystal lattice and its realization is presented. Section 3 is devoted to the theory of vibrations of a crystal lattice. Finally, in section 4 the algebraic formalism of hearing the eigenvalues of Laplacian on the torus \( \mathbb{R}^n/L \) is provided and some special cases are studied.

2. Crystal Lattices

In this section we follow the Sunada’s graph theory method to introduce the notion of a crystal graph [5].

2.1. Graphs and crystals

A graph is an ordered pair \( X = (V, E) \) of disjoint sets \( V \) and \( E \) with two maps \( o : E \rightarrow V \) and \( t : E \rightarrow V \). It is finite if both \( V \) and \( E \) are finite sets. A geometric graph is \( V \cup (E \times [0, 1]) / \sim \) where the equivalence relation \( \sim \) is defined by \( o(e) \sim (e, 0), t(e) \sim (e, 1) \). Let \( X \) and \( X_0 \) be two geometric graphs and let \( \pi : X \rightarrow X_0 \) be a covering map. The graph \( X \) is called an abelian covering space of \( X_0 \) if the deck transformation group is abelian. An abstract crystal \( C \) is an infinite regular covering of a geometric graph \( X \) over a finite graph \( X_0 \), with free abelian deck transformation group. Every abstract crystal is obtained by choosing a subgroup \( H \) of the homology group \( H_1(X_0, \mathbb{Z}) \) when \( \frac{H_1(X_0, \mathbb{Z})}{H} \) is a free abelian group.

2.2. Realization

Set \( l^2(V) = \{ f : V \rightarrow \mathbb{C} | \sum_{x \in V} |f(x)|^2 < \infty \} \).

**Definition 2.1.** The discrete Laplacian \( \Delta : l^2(V) \rightarrow l^2(V) \) is defined by

\[
\Delta(f)(x) = \sum_{e \in E, o(e) = x} (f(t(e)) - f(o(e))).
\]
Definition 2.2. *(Periodic realization)* A piecewise linear map $\phi : X \to \mathbb{R}^n$ is said to be a periodic realization, if there exists an injective homomorphism $\rho : L \to \mathbb{R}^n$ such that

a) $\phi(\sigma x) = \phi(x) + \rho(\sigma)(x \in V, \sigma \in L)$ and b) $\rho(L)$ is a lattice subgroup of $\mathbb{R}^n$.

The periodic realization $\phi : X \to \mathbb{R}^n$ is harmonic (or standard in the Sunada’s notation) provided that it is a solution of the discrete Laplace equation $\Delta \phi = 0$ and there exists a positive constant $c$ such that

$$\sum_{e \in X_0} x.(\phi(t(e')) - \phi(o(e')))(\phi(t(e')) - \phi(o(e'))) = cx, \forall x \in \mathbb{R}^n$$

where $e' \in \pi^{-1}(e)$ is arbitrary (maximal orthogonality property).

3. Vibration of lattices

Harmonic realization of a lattice is the state of minimum energy of its realizations which depends on the function $\rho : L = \frac{H_1(X_0,\mathbb{Z})}{H} \to \mathbb{R}^n$ as the symmetries of the covering space $\pi : X \to X_0$. In crystallography it is assumed that two elements (atoms) in the same orbit of $\rho(L)$ are of the same type. At temperatures close to zero a crystal lattice vibrates about its equilibrium position (its harmonic realization) by effect of its inter-atomic forces. The motion $f$ satisfies the equation

$$\frac{d^2(f)}{dt^2} = Df$$

where $D$ is the discrete elastic Laplacian defined by

$$Df(x) = \frac{1}{m(x)} \sum_{e \in E_x} A(e)(f(t(e)) - f(o(e)))$$

for positive definite symmetric $m \times m$ matrices $A(e)$ (this is an extra, but useful condition), $m = card(E_0)$, and masses $m(x)$ associated to atoms $x \in V$. Physicists call $A$, the matrix of atomic force constants. $D$ is an $L$-equivariant linear bounded self-adjoint operator on the Hilbert space generated by the space $C(V, \mathbb{C}^n)$ equipped with the inner product $\langle f, g \rangle = \sum_{x \in V} f(x).g(x)m(x)$. 

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3.1. Hamiltonian formalism of the motion equation

In this section a Hamiltonian formalism is used to provide a decomposition of a vibration to simpler harmonic vibrations \[4\]. Let \( w : l^2(V, m) \times l^2(V, m) \to \mathbb{R} \) be a symplectic form on \( l^2(V, m) = \{ \sum_{x \in V} |f(x)|^2 m(x) < \infty \} \) defined by \( w(u, v) = \text{Im} < u, v > = \text{Im} (\sum_{x \in V} u(x)v(x)m(x)) \). Let \( H(u) = \frac{1}{2} < -D, u, u > \). Let \( \hat{L} \) be the unitary character group of \( L \), and \( d\chi \) denotes the normalized Haar measure on \( \hat{L} \). Then the Bloch decomposition of the Hamiltonian system \((l^2(V, m), w, H)\) is

\[
(l^2(V, m), w, H) = \bigoplus \int_{\hat{L}} (l^2(V, m)_\chi, w_\chi, H_\chi) d\chi, \tag{5}
\]

where \( l^2(V, m)_\chi = \{ u \in l^2(V, m)|u(\sigma x) = \chi(\sigma)u(x), \forall \sigma \in L \} \). In fact, the elements \( \chi \in \hat{L} \) are the same as the angular frequencies. Using the index \( \chi \) for an operator means that we restrict its domain to the vector space \( l^2(V, m)_\chi \). Note that we have a decomposition of \( D \) as \( \int_{\hat{L}} D_\chi d\chi \). The operators \( -D_\chi, \chi \neq 1 \) are positive definite. Zero is an eigenvalue of \( D_1 \) of multiplicity \( n \) with constant eigenfunctions.

For the eigenmodes (eigenfunctions) corresponding to the first \( n \) eigenvalues of \( D_\chi \), neighboring atoms move in phase with each other with the same amplitude and each of which is called an \textbf{acoustic phase}. The velocity of these phases is called the acoustic phase velocity. It is equal to \( \frac{1}{\sqrt{2\pi\|\chi\|^2}} s_i(\chi), \ i = 1, ..., n \), where one can prove

\textbf{Theorem 3.1.} \( s_i(\chi)^2 \) \( (i = 1, \ldots, n) \) are eigenvalues of the symmetric matrix

\[
A_\chi := \frac{2\pi^2}{m(V_0)} \sum_{e \in E_0} (\chi . v(e))^2 A(e). \tag{6}
\]

In particular, \( s_i(\chi)^2 > 0 \) for \( \chi \neq 0 \) \[4\].

In the previous theorem \( m(V_0) \) is the sum of masses of vertices of \( X_0 \) (the \textbf{cell mass of crystal}).

4. Laplacian on tori

For simplicity denote \( \rho(L) \) also by \( L \). The character group of the lattice \( L \) is equal to the torus \( \hat{L} = \frac{\mathbb{R}^n}{L^*} \) where \( L^* \) is the reciprocal lattice of \( L \), i.e
Equip each of these tori with the natural Euclidean metric. The length of closed geodesics of $\hat{L}$ are the same as the eigenvalues of the Laplace-Beltrami Operator on the torus $\frac{\mathbb{R}^n}{L}$. Let us integrate $s_i(\chi)^2$ over simple closed geodesics including 1. We call this the integrated acoustic velocity. A natural question arising here is:

**What is the relation between integrated acoustic velocity of the crystal lattice $C$ and the Laplacian eigenvalues of the torus $\frac{\mathbb{R}^n}{L}$?**

4.1. Algebraic formalism

Even though, there are many choices leading us to diverse nice problems about the acoustic phase velocity and the spectrum of the symmetric torus, in this subsection we only investigate the integration of $\sum_{i=1}^{n} s_i(\chi)^2$. Let $T$ denote the set of all simple closed geodesics of $\hat{L}$ initiated from the identity and parametrized by the interval $[0,1]$.

**Definition 4.1.** The integrated acoustic phase velocity on $c \in T$ is defined by $\int_c \sum_{i=1}^{n} s_i(\chi)^2 d\chi$.

**Definition 4.2.** The integrated acoustic spectrum of a crystal lattice $C$ is defined by the set

$$\left\{ \int_c \sum_{i=1}^{n} s_i(\chi)^2 d\chi | c \in T \right\}.$$ 

(8)
We may pay to the next question:
When can we hear the spectrum of the torus $\mathbb{R}^n/L$ from the acoustic spectrum of the crystal lattice $C$? (**)

**Theorem 4.3.** Consider $m$ vectors $v_i = v(e_i), i = 1, \cdots, m$ where $v(e_i) = \phi(t(e_i)) - \phi(e(e_i))$. Assume $|v_i| = 1$ and $\text{tr} A(e_i) = \frac{3}{2\pi^2} m(V_0), i = 1, \cdots, m$.
Then the acoustic spectrum is equal with $\text{Asp} = \left\{ \sum_i (\chi.v_i)^2 | \chi \in L \right\}$.

Proof: The theorem is a result of the fact that the summation $\sum_{i=1}^n s_i(\chi)^2$ is the trace of the matrix $A_{\chi}$ (Theorem 3.1) and the fact that $\int \sum_{i=1}^n s_i(t)^2 dt = \sum_{i=1}^n \int_0^1 s_i(t)^2 dt = \int_0^1 t^2 s_i(t)^2 dt = \frac{2\pi^2}{3 m(V_0)} \sum e_{E_0}(\chi.v(e_i))^2 tr A(e_i)$.

The problem (**) can be written as follows,
Let $\text{Asp} = \left\{ \sum_i (\chi.v_i)^2 | \chi \in L \right\}$, can we determine the set $\text{Lsp} = \{||\chi|| | \chi \in L\}$?

**Theorem 4.4.** Under the assumptions of Theorem 4.3, the $\text{Asp}$ determine the lengths of elements of $L$ and $L^*$ up to a constant $c$.

Proof: According to the property 2 of a standard realization, $\sum_i (\chi.v_i)^2 = c |\chi|^2$. On the other hand from the Poisson formula we have $\sum_{y \in L^*} e^{-4\pi^2|y|^2 t} = \frac{\text{Volume}(L)}{(4\pi t)^\frac{n}{2}} \sum_{s \in L} e^{-|s|^2/4t}$ which provides the relation between lengths of elements of $L$ and $L^*$.

The physical interpretation of Theorem 4.4 is that when the average of quantities $(A(e)x.x)$ on the unit sphere (which is a divergence like quantity) are the same for neighboring atoms and the crystal lies in its harmonic position, the integrating of velocities $(s_i(\chi))$ of independent acoustic phases over the closed geodesics of the angular momentum phase space determine the length of elements of the symmetric lattice of the crystal up to a constant.

4.2. Generalized problem

In this subsection we consider examples for a more general case. We ignore that the set of vectors $v_i, i = 1, \cdots, n$ are obtained from a lattice harmonic embedding. Moreover we assume some extra assumptions about our lattice.

Example 1: Let $v_1, v_2, v_3$ be an orthogonal basis of $\mathbb{R}^3$ and $v_4$ makes angle $120^\circ$ with each vector $v_1, v_2, v_3$. Also let the position of $v_4$ is such that $\chi.v_4 \in \mathbb{Q}^c$ for $\chi \in L$. Then the set $\text{Asp}$ is equal to $\{||\chi||^2(1 + \cos^2 \theta_{i\chi}) | \chi \in L \}$ where $\cos^2 \theta_{i\chi}$ is irrational for all $\chi \in L$ which denotes the angle between $\chi$ and $v_4$.

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We can obtain candidates for $L_{sp}$’s by dividing each element of the set $Asp$ by the numbers in the interval $(1, 2)$ which generate integer numbers and then computing the square root of them.

Example 2: In this example let us conceive some extra knowledge about $L$ and the vectors $v_i$, $i = 1, \cdots, n$. Suppose we know there are four basic atoms in each cell of a crystal and one of them is joined with the others. Therefore, we have three vectors and assume they have the same length 1. Furthermore suppose that there is a number $k$ such that $kL$ is an integral lattice generated by two vectors of the same length. Concisely let $L = \{k\chi + l\eta : k, l \in \mathbb{Z}\}$ and $|\eta| = |\chi|$. By these conditions we have

$$Asp = |\chi|^2\{k^2(\sum_{i=1}^{3}\cos^2\theta_{i\chi}) + l^2(\sum_{i=1}^{3}\cos^2\theta_{i\eta}) + 2kl(\sum_{i=1}^{3}\cos\theta_{i\chi}\cos\theta_{i\eta})|k, l \in \mathbb{Z}\},$$

where $\theta_{i\chi}$ and $\theta_{i\eta}$ are respectively the angles of $v_i$ with $\chi$ and $\eta$. Assume that $\sum_{i=1}^{3}\cos\theta_{i\chi}\cos\theta_{i\eta}$ be a positive number, then the minimum of the set $\frac{T}{|\chi|^2}$ is equal to

$$\min\{\sum_{i=1}^{3}\cos^2\theta_{i\chi}, \sum_{i=1}^{3}\cos^2\theta_{i\eta}\}.$$

Now, assume that we know all solutions of the next algebraic problem.

Problem. Let $\mathbb{Z} \ast \mathbb{Z} = \{x^2 | x \in \mathbb{Z}\}$ and $\mathbb{Z}.\mathbb{Z} = \{x.y | x, y \in \mathbb{Z}\}$. Suppose that $m \in \mathbb{Z}$, $\alpha, \beta, \gamma \in \mathbb{R}^+$, and assume that we know the set $M = \{m(\alpha\mathbb{Z} \ast \mathbb{Z} + \beta\mathbb{Z} \ast \mathbb{Z} + \gamma\mathbb{Z} \ast \mathbb{Z})\}$. Find all four tuple $(m, \alpha, \beta, \gamma)$ with the same $M$.

For each 3 tuples $(\alpha, \beta, \gamma)$ we must find the set of solutions for the set of equations

$$\sum_{i=1}^{3}\cos^2\theta_{i\eta} = \beta, \sum_{i=1}^{3}\cos\theta_{i\chi}\cos\theta_{i\eta} = \gamma, \sum_{i=1}^{3}\cos^2\theta_{i\chi} = \alpha.$$

A simple geometric discussion on the angles provide a description of the set $L_{sp}$.

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