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Proving a measure of lattice differences

Lawrence C. Andrews[a]* and Herbert J. Bernstein[b]

[a]Ronin Institute, 9515 NE 137th St, Kirkland, WA, 98034-1820 USA, and [b]Ronin Institute, c/o NSLS-II, Brookhaven National Laboratory, Upton, NY, 11973 USA.

E-mail: larry6640995@gmail.com

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Abstract

Abstract Unit cells

Note: In his later publications, Boris Delaunay used the Russian version of his surname, Delone.

1. Introduction

A recent article (Bright *et* al., 2023) questioned the formal basis of the measures of differences between lattices that are described by Andrews & Bernstein (2023) (and references therein).

Here we present a formal description of the above mentioned methods.

2. Finding a minimum distance

Consider some metric space **X** in which a distance can be determined between any two objects in **X**.

A distance in **X** is defined as

$d = \mid \mathbf{x}\text{-}\mathbf{y} \mid$ for $\mathbf{x},\mathbf{y} \in \mathbf{X}$.

The question that immediately arises how to represent the object in **X**. The conventional choices are to choose either the basis vectors of the lattice, a description of the unit cell itself, or as objects in some space, such as ...

The points in lattices in 2 dimensions are addressed by the operations of the "modular group", also named PSL(2,**Z**). The corresponding 3 dimensional group is PSL(3,**Z**).

Invariants are known for lattices in two dimensions (see Jones & Singerman (1987), page 176 and following). Bright *et* al. (2023) have considered alternatives. However, invariants are not known for PSL(3,**Z**) or in higher dimensions.

To compute the distance between two lattices (represented in a metric space, with operators g_i in the group **G**), we define

$d_{min} = \min \left| g_i\mathbf{y} - \mathbf{x} \right|$ for $\mathbf{x},\mathbf{y} \in \mathbf{X}$ and $\mathbf{g_i} \in \mathbf{G}$.

We conjecture that

$dy_{min} = \min \left| g_i\mathbf{x} - \mathbf{y} \right|$ for $\mathbf{x},\mathbf{y} \in \mathbf{X}$ and $\mathbf{g_i} \in \mathbf{G}$.

has the same value as d_{min} above.

3. Computing the minimum distance

While Section 2 contains a definition for a minimum distance, a problem still exists. The group $PSL(3, \mathbf{Z})$ is an infinite group. For practicality, a finite algorithm is required.

The first step is compute the distance between the two points of interest with g_i as the identity operation. From the group **G**, a set of operators must be chosen. It should include those operations that do not change the norm of the affected point plus a sufficient set of the other operations. The generators of the **G** is a minimal set, but for efficiency an expanded set is useful.

The above set of operations must then be applied iteratively until the distance between the two points exceeds some limit.

4. Summary

Summary blah blah blah

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Synopsis

Unit cells