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Finite motions from periodic frameworks with added symmetry

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ABSTRACT

Recent work from authors across disciplines has made substantial contributions to counting rules (Maxwell type theorems) which predict when an infinite periodic structure would be rigid or flexible while preserving the periodic pattern, as an engineering type framework, or equivalently, as an idealized molecular framework. Other work has shown that for finite frameworks, introducing symmetry modifies the previous general counts, and under some circumstances this symmetrized Maxwell type count can predict added finite flexibility in the structure.

In this paper we combine these approaches to present new Maxwell type counts for the columns and rows of a modified orbit matrix for structures that have both a periodic structure and additional symmetry within the periodic cells. In a number of cases, this count for the combined group of symmetry operations demonstrates there is added finite flexibility in what would have been rigid when realized without the symmetry. Given that many crystal structures have these added symmetries, and that their flexibility may be key to their physical and chemical properties, we present a summary of the results as a way to generate further developments of both a practical and theoretic interest.

1. Introduction

The theory of periodic frameworks has undergone rapid and extensive development in the last 4 years (Borcea and Streinu, 2010a,b; Malestein and Theran, 2010; Ross, 2011). We now have necessary conditions (call them Maxwell counts) for such frameworks to be rigid, either with a fixed lattice of translations or with a flexible lattice of translations. Underlying much of the recent work are finite 'lattice rigidity matrices' for the equivalence classes of vertices and edges under the infinite group of translations $\mathbb{Z}^d$ in d-space. With the corresponding count of periodicity-preserving trivial motions under these constraints (typically d translations), the number of rows, e, and columns, $dv + l$ (where l is the number of lattice parameters) of these 'orbit matrices' lead to necessary Maxwell type counts for a framework to be infinitesimally rigid (Borcea and Streinu, 2010a; Malestein and Theran, 2010; Ross, 2011): $e \geqslant dv + l - d$.

The theory of finite symmetric frameworks has also experienced some breakout results, building on a decade or more of initial Maxwell type necessary conditions for frameworks of various symmetry groups (Fowler and Guest, 2000; Guest and Fowler, 2007; Connelly et al., 2009). In some key cases, these symmetry conditions predict finite motions for frameworks realized generically within the symmetry constraints, but whose graphs would be generically rigid without symmetry (Kangwai and Guest, 1999; Bricard, 1897). Recently, key results of this work have been expressed in terms of 'orbit rigidity matrices' for the equivalence classes of vertices and edges under the group of symmetry operations $\mathcal{S}$ (Schulze, 2009, 2010d; Schulze and Whiteley, 2010). With modified counts for the symmetry-preserving trivial motions $t_{\mathcal{S}}$, and with e_0 and v_0 denoting the number of edge orbits and vertex orbits under the group action of $\mathcal{S}$, respectively, these matrices lead to Maxwell type necessary counts for frameworks to be infinitesimally rigid: $e_0 \geqslant dv_0 - t_{\mathcal{S}}$.

Given that many crystal structures combine both periodic structure and symmetry within the unit cells, it is natural to investigate the interactions of these two types of group operations. So we will consider frameworks with 'combined symmetry groups' of the form $\mathbb{Z}^d \rtimes \mathcal{S}$, where $\mathbb{Z}^d$ is the group of translations of the framework, $\mathcal{S}$ is the group of additional symmetries of the framework, and $\rtimes$ denotes the semi-direct product of $\mathcal{S}$ acting on $\mathbb{Z}^d$. Note that every symmetry operation in such a group can be written as a unique product of an element of $\mathbb{Z}^d$ and an element of $\mathcal{S}$. However, since $\mathcal{S}$ is typically not normal in $\mathbb{Z}^d \rtimes \mathcal{S}$, the groups $\mathbb{Z}^d \rtimes \mathcal{S}$ are in general not direct products. Details on the semi-direct product can be found in any abstract algebra text, such as Dummit and Foote (1991). In Section 6 we will introduce combined 'orbit matrices' for the groups $\mathbb{Z}^d \rtimes \mathcal{S}$. Combined with the counts of the trivial mo-

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