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A General Algorithm for Calculating Irreducible Brillouin Zones

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Abstract. Calculations of properties of materials require performing numerical integrals over the Brillouin zone (BZ). Integration points in density functional theory codes are uniformly spread over the BZ (despite integration error being concentrated in small regions of the BZ) and preserve symmetry to improve computational efficiency. Integration points over an irreducible Brillouin zone (IBZ), a rotationally distinct region of the BZ, do not have to preserve crystal symmetry for greater efficiency. This freedom allows the use of adaptive meshes with higher concentrations of points at locations of large error, resulting in improved algorithmic efficiency. We have created an algorithm for constructing an IBZ of any crystal structure in 2D and 3D. The algorithm uses convex hull and half-space representations for the BZ and IBZ to make many aspects of construction and symmetry reduction of the BZ trivial. The algorithm is simple, general, and available as open-source software.

AMS subject classifications: 68U05, 20H15, 52B55, 52C07, 68W40, 57Z05, 57Z15

Key words: Brillouin zone, irreducible Brillouin zone.

1 Motivation

Computing intrinsic properties of materials using density functional theory requires numerical integration [1]. For example, the energy of the electrons (band energy) and the number of electrons in a given energy state (density of states) are properties of materials that are obtained by numerical integration. The domain of integration for these integrals is a Voronoi cell called the first Brillouin zone (referred to throughout this paper as simply

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Figure 1: The Brillouin zone for a body-centered tetragonal lattice. The Brillouin zone is the integration domain of integrals that give properties of materials. It is also a convex polygon that often has a complicated shape. This plot, and many others in this article, were created with SymmetryReduceBZ (see `https://github.com/jerjorg/SymmetryReduceBZ.jl`).

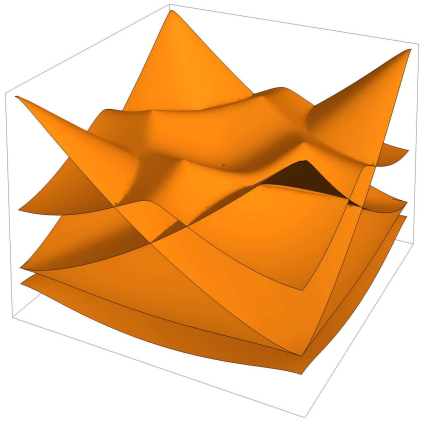

Figure 2: The electronic band structure or algebraic surface of a 2D toy model of a material. The band structure is often the integrand for integrals that give properties of materials. A band structure in 2D was chosen due to the difficulty of visualizing in more than 3D. The Brillouin zone in this case is simply a square.

Brillouin zone or BZ). A Voronoi cell is the region of space closer to one point in a mesh than to any other point in the mesh. In terms of geometry, the BZ is a convex polyhedron that often has a complicated shape. The integrand for the band energy or density of states is a periodic, algebraic surface called the electronic band structure. An example BZ for a 3D lattice is shown in Fig. 1, and the electronic band structure for a 2D toy model is shown in Fig. 2.

The electronic band structure is computationally expensive to evaluate because each evaluation means solving an eigenvalue problem of a Hermitian matrix of order from hundreds to thousands. The number of evaluations is reduced by up to a factor of 48 by using the symmetry of the material, which allows one to reuse eigenvalues. In other words, if two points are symmetrically equivalent (for example, a rotation by 90° maps one point to the other), the eigenvalues are identical at both points.