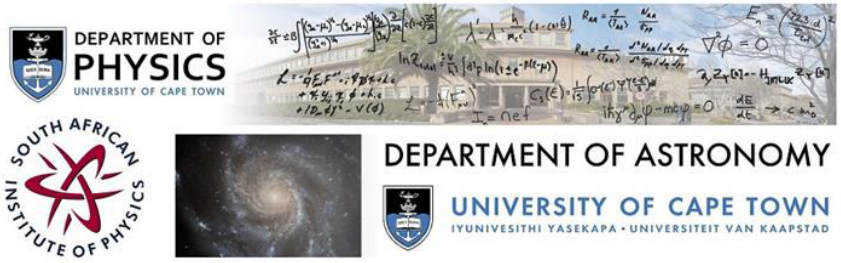

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Visualizing higher order Brillouin zones with applications

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Abstract content
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It is common for students to use modern electronic structure codes (ESC) as black-boxes, with little conceptual understanding of the underlying theoretical and computational details of the main components involved. What is needed are simplified problems that illustrate these concepts and are easily coded by third year undergraduate students. An important concept in solid state physics is the first Brillouin zone (BZ) which uniquely determines the electronic energies and wavefunctions for electrons in a periodic potential. ESC calculate material properties using integrations over this zone. Higher order zones are also important; the BZ boundaries define Bragg planes and the constant energy Fermi surface sometimes extends into these zones. The shape of this surface is important in determining many metal properties and low energy interactions.

Using a simple algorithm to sort k-points into their respective Brillouin zones, we can visualize a BZ of any order as well as deconstruct the Fermi surface for metals when it extends into the higher order zones. This is pedagogically useful as a student can write a small code, in a language of their choice, to implement the algorithm for any crystal lattice. We present results for 2D and 3D.

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Primary author: Dr ANDREW, Richard (University of Pretoria)

Co-authors: Prof. CHETTY, Nithaya (University of Pretoria); Dr SALAGARAM, Trisha (University of Cape Town)

Presenter: Dr SALAGARAM, Trisha (University of Cape Town)

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