CENTER FOR COMPUTATION & TECHNOLOGY

Interdisciplinary | Innovative | Inventive

LOUISIANA STATE UNIVERSITY

Events

Current Events
Lectures▼
Events Archive▼

Computational Mathematics Seminar Series

Convergence of the Planewave Approximations for Quantum Incommensurate Systems

Daniel Massatt, Louisiana State University

Assistant Professor

Digital Media Center 1034
February 07, 2023 - 03:30 pm

Abstract:

Incommensurate structures arise from stacking single layers of low-dimensional materials on top of one another with misalignment such as an in-plane twist in orientation. While these structures are of significant physical interest, they pose many theoretical challenges due to the loss of periodicity.

In this paper, we characterize the density of states of Schrödinger operators in the weak sense for the incommensurate system and develop novel numerical methods to approximate them. In particular, we (i) justify the thermodynamic limit of the density of states in the real space formulation; and (ii) propose efficient numerical schemes to evaluate the density of states based on planewave approximations and reciprocal space sampling.

We present both rigorous analysis and numerical simulations to support the reliability and efficiency of our numerical algorithms.

Speaker's Bio:

Daniel Massatt is an Assistant Professor in the Mathematics Department at Louisiana State University. He received his Ph.D degree in Mathematics at the University of Minnesota in 2018. His research includes electronic structure of materials including incommensurate layered 2D materials and topological insulators, multiscale modeling, and numerical analysis.