復旦大學
FUDAN UNIVERSITY

Applied Math Ph.D. Seminar

Decay Properties of Hamiltonian Transformation with Applications to Band Structure Calculation

Speaker: Kai Wu (University of Science and Technology of China)

Time: 2022-03-03, 16:10 to 17:00

Location: Rm 1801, Guanghua East Tower

Mentor: Jinlong Yang and Wei Hu (University of Science and Technology of China)

Abstract: We propose a new method to calculate band structure of quantum systems. It constructs the quasi-Hamiltonian matrix using several eigenvalues and corresponding eigenvectors at the uniform k-point grids, then performing Fourier interpolation to obtain the quasi-Hamiltonian at any k-point. We find some invertible transformations make the quasi-Hamiltonian matrix decays faster in real space, which generates more accurate band structures. The decay properties of Hamiltonian transformation associated with both sparse and dense Hamiltonian matrices can be described by an inequality using approximation theory and matrix analysis. In the sparse matrix case, we can simplify the inequality and estimate the decay property analytically. In the dense matrix case, the inequality is more complicated and is studied numerically.