

凝縮系物理学ゼミナール

Condensed Matter Theory Seminar

Date: 13:30-15:00, Wednesday, 14, May 2025

Title: Electronic and Magnetic Structures of UTe_2

Speaker: Dr. Makoto Shimizu

Language: English

Abstract:

The heavy-fermion paramagnetic superconductor UTe_2 has been extensively studied as a strong candidate for spin-triplet superconductivity. Early studies suggested the presence of ferromagnetic fluctuations, which were considered a potential pairing mechanism for spin-triplet Cooper pairs. However, neutron scattering experiments have revealed antiferromagnetic fluctuations instead. Some theoretical works propose that spin-triplet pairing may be mediated by these antiferromagnetic fluctuations. Nevertheless, more realistic models incorporating sublattice, orbital, and spin degrees of freedom are required to fully understand the magnetic structure and pairing mechanism.

In this study, we investigate the electronic and magnetic structures of UTe_2 . We begin with first-principles calculations based on density functional theory (DFT) including spin-orbit coupling. Using symmetry-conserving projected Wannier functions, we construct a 72-band tight-binding model comprising U 5f, U 6d, and Te 5p orbitals. At the Fermi level, the U 5f ($j = 5/2$) orbitals dominate the density of states. Focusing on these orbitals, we calculate the irreducible susceptibility. In this seminar, I will present the calculated spin susceptibility and discuss its comparison with experimental results.

References:

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- [3] D. Aoki *et al.*, J. Phys. Soc. Jpn. **89**, 053705 (2020).
- [4] S. Ran *et al.*, Phys. Rev. B **101**, 140503 (2020).
- [5] W. Knafo *et al.*, arXiv:2311.05455.
- [6] M. Shimizu, and Y. Yanase, arXiv:2408.04292.