Master thesis project

at the Institute of Theoretical and Computational Physics, TU Graz

Correlation effects in 2D quantum materials

Quantum materials with a 2D structure, such as **transition-metal dichalcogenides (TMDs)**, can host phases ranging from Mott insulating to superconducting and quantum spin liquids. Predicting their properties requires advanced electronic structure and diagrammatic techniques. In this project, we will investigate 1T-TaS(e)₂, a strongly correlated TMD, to determine whether it hosts a **quantum spin liquid** state, where spins remain disordered even at the lowest temperatures. Our approach will combine density functional theory with diagrammatic methods, computing **spin susceptibilities** using the ab-initio dynamical vertex approximation.



Crystal structure of TMDs

Helpful prerequisites: good knowledge in quantum mechanics and linear algebra, programming skills (Python, Fortran).

What you will learn: skills in high-performance computing, participation in a cutting-edge research project in theoretical solid-state physics.

Employment: student assistant for 6 months (8h/week).

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