

Master thesis projects 2023

Condensed Matter Theory Group, Prof. Titus Neupert

Excitons in moiré pattern (with Glenn Wagner)

When two waves with slightly different frequencies are superimposed, interference between the two waves leads to a modulation of the amplitude of the wave in time. This phenomenon is known as a beat pattern and it is a familiar phenomenon in acoustics. The equivalent phenomenon in real space instead of in time is known as a moiré pattern. It occurs when two lattices with slightly different lattice constants are superimposed. Materials with a moiré structure have been attracting a lot of attention recently, notably due to the observation of unconventional superconductivity.

In this project we will investigate transition metal dichalcogenide bilayers. Since the bilayers are built up from materials with different lattice constants, this results in a moiré pattern and it is known that one then obtains Chern bands, much like the Landau levels in the quantum Hall effect. We will investigate excitons (bound states of particles and holes) in these Chern bands in order to determine whether they can exhibit a bosonic fractional quantum Hall effect.

This will be a numerical project involving exact diagonalization.

Interacting topological quantum chemistry (with Martina Soldini)

Crystalline materials where interactions between electrons are negligible have been successfully classified, based on their band structure, by means of the ‘topological quantum chemistry’ theory, which allows to identify topological phases of matter within these materials. We have recently developed a theoretical framework called ‘interacting topological quantum chemistry’, an extension of the (non-interacting) ‘topological quantum chemistry’ approach to the interacting realm, which relies on n-body Green’s function to classify interacting many-body states. We considered gapped, non symmetry broken, and time reversal symmetric many-body ground states of itinerant electrons, and we proposed a classification scheme for some classes of these interacting states that relies on the symmetries of their n-body Green’s function.

With the project proposed here, we want to connect the tools developed for electronic systems to the case of spin-models, corresponding to a low-energy description of the initial Mott insulators. This would amount to first constructing and studying a specific spin model and its correlation functions, and then bridging the results obtained in the spin model to the known results in the electronic case to characterise the spin state. This project involves both analytical work, in particular involving many-body methods in condensed matter theory and tools from group theory, as well as a numerical part in the implementation of spin models and the evaluation of spin correlation functions.

Microscopic investigation of the upper critical field of a superconductor (with Bernhard E Lüscher)

The coupling of an external magnetic field to the electrons in a material may destroy the superconducting state through Zeeman coupling or the coupling to the electrons’ orbital motion. The latter coupling, often the relevant contribution, can be introduced through minimal coupling or, on the level of a tight-binding description, through Peierl’s substitution and will gradually decrease the transition temperature. The question arises at which critical field H_{c2} a material’s critical temperature reaches zero. This critical field is of interest both from an applied as well as from a fundamental perspective—the magnitude of H_{c2} and the shape of the transition line can give insights into the microscopic details of the superconducting order parameter.

The starting point of this project is a tight-binding Hamiltonian on a square lattice including a pairing-interaction term. Both analytical and numerical approaches will be required to arrive at and eventually solve a self-consistency equation for the order parameter and consequently, the critical temperature. In a further step, multiple orbitals or different couplings to the magnetic field, for example Zeeman coupling, can be included. Such complications will be crucial to understand the magnetic-field–temperature phase diagram of superconductors of current interest, like Sr_2RuO_4 , 4Hb-TaS_2 , or CeRh_2As_2 . Ultimately, we want to work towards crafting a numerical tool to find the upper critical field for arbitrary functional forms of the order parameter and complicated band structures.