CSC-RUB PhD Project Proposal

Title: Functional renormalization group approach to strongly correlated moiré materials

Sector of research: Theoretical solid-state physics, strongly correlated materials

Degree awarded: Dr. rer. nat. (PhD)

Keywords: Strongly correlated electrons, unconventional superconductivity, competing instabilities, moiré materials, condensed-matter field theory, functional renormalization group

Supervisor of PhD project: Prof. Dr. Michael Scherer, Faculty of Physics and Astronomy, Ruhr University Bochum, E-Mail: scherer@tp3.rub.de; ORCID: 0000-0003-0766-9949

Research focus of supervisor: The research of our group is focused on the exploration of emergent phenomena and correlated behavior of quantum matter and quantum materials. We develop and employ modern quantum field theoretical methods to understand and predict novel effects in a broad field ranging from condensed matter to particle physics. Recently, a strong focus of our research has been the investigation of strongly correlated states, e.g., different forms of magnetism and unconventional (topological) superconductivity in novel moiré materials, such as twisted bilayer graphene and related transition metal dichalcogenides. To that end we develop and apply functional renormalization group methods to access both, the universal (quantum) critical behavior as well as the non-universal Fermi-surface instabilities and phase diagrams of such materials systems. The goal of our research is to identify and quantitatively describe exotic states of matter in realistic models of novel materials and to inspire future experiments.

Publications:

1) Realization of nearly dispersionless bands with strong orbital anisotropy from destructive interference in twisted bilayer MoS2,
   L. Xian, M. Classen, D. Kiese, M. M. Scherer, S. Trebst, D. M. Kennes, A. Rubio,

2) Universal principles of moiré band structures,
   J. Attig, J. Park, M. M. Scherer, S. Trebst, A. Altland, A. Rosch,

3) Competing orders at higher order Van Hove points,
   L. Classen, A. V. Chubukov, C. Honerkamp, M. M. Scherer,

4) Competing phases of interacting electrons on triangular lattices in moiré heterostructures,
   L. Classen, C. Honerkamp, M. M. Scherer,

5) Four-loop critical exponents for the Gross-Neveu-Yukawa models,
   N. Zerf, L. N. Mihaila, P. Marquard, I. F. Herbut, M. M. Scherer,

H-index of the last 5 years: 26 Number of publications in the last 5 years: 27

Second Supervisor of PhD project: Prof. Dr. Ilya Eremin, Faculty of Physics and Astronomy, Ruhr University Bochum, E-Mail: Ilya.Eremin@ruhr-uni-bochum.de; ORCID: 0000-0003-0557-8015
### Summary of research plan

**Background:** In 2018 correlated insulating, superconducting and strange metal behavior have been observed in twisted bilayer graphene. In the experimentally studied systems two stacked sheets of graphene are twisted by a small rotational angle, giving rise to a moiré interference pattern with more than 10,000 atoms per unit cell. The emergence of interaction-induced correlated states has since generated tremendous research activity in various moiré materials launching the novel field of twistronics. The theoretical description of correlated behavior in moiré materials employing many-body methods faces new challenges going far beyond the conventional Hubbard model paradigm, including complex electronic multi-band structures, large Coulomb matrix elements, and interplay with enhanced electron-phonon couplings.

Understanding correlation effects is key for the successful development of this thriving field and therefore the development and application of powerful new theoretical approaches is mandatory. With the functional renormalization group technologies developed in my group, we have laid the field-theoretical groundwork for such descriptions.

**Study objective:** The objective of the PhD project is to further develop analytical aspects and the numerical implementation of the functional renormalization group approach to correlated fermion systems and apply it to novel moiré materials, including transition metal dichalcogenides and graphene-based systems. The resulting phase diagrams will predict and characterize the correlated states of matter of moiré materials and guide future experiments.

**Expected Results:** Based on the groundwork already provided in my group, a smooth start of the PhD project is secured. The PhD candidate will further develop the method to apply it to novel moiré systems that are under current experimental investigation. Publications in high-ranking journals will be realized.

**Methods:** Quantum field theory, condensed-matter field theory, solid state physics, functional renormalization group, numerical implementation of the functional renormalization group. Required computer hardware (access to a cluster, workstation, etc.) and software (Julia, Python, C++) will be provided.

**Candidate Requirements:** Candidates should have studied theoretical physics on the MSc level and have a very strong background in quantum field theory, solid state physics, condensed-matter field theory, basics of the renormalization group. They should also have very good coding skills in Julia, Python, C++ or similar. Candidates are expected to be able to work independently as well as in a team with other PhD students and postdocs. Good English language skills are required.

**Motivation for CSC application** (max 250 words): The research of our group is focused on the exploration of emergent phenomena and correlated behavior of quantum matter and quantum materials. To that end, we develop and employ cutting-edge quantum field theoretical methods to understand and predict novel effects in a broad field ranging from condensed matter to particle physics. Our group maintains active cooperations with researchers in Canada, China, Denmark, Great Britain, the United States, and throughout Germany. Furthermore, we are a member of the Cologne-based collaborative funding initiative Control and Dynamics of Quantum Materials (CRC1238), which offers many seminars and workshops in the relevant research field. Also, the CRC1238 provides additional funding opportunities for travels to PhD students. Furthermore, the project will be embedded in the Ruhr-University Research School, which offers additional soft-skill seminars, tutoring, and career development.