1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Simulation quantum many-body problems on moiré superlattices

1.1. Project goals

The aim of this project is theoretical investigation of twisted two-dimensional crystals, which are new quantum simulators. Moiré superlattices formed in this way characterize by high tunability, showing the feasibility to realize and control a large number of fundamental many-body quantum models relevant in the field of condensed matter physics. Different choices of two-dimensional (2D) heterostructure compositions twisted by different angles can realize a wide range of effective low-energy electronic tight-binding Hamiltonians with various geometries, topology, and interactions beyond the Hubbard model, including long-range Coulomb interactions that can be also screened in a controllable manner. A key characteristic of moiré quantum materials is the presence of tunable flat bands, which allow to control relative interaction strength to kinetic energy. Our goal is to determine type of materials and conditions for observation magnetic or correlated phases in order to direct future experiments. We will investigate and analyse theoretically electronic properties of many twisted heterostructures and confront our results with the latest experiments.

1.2. Outline

In 2018, MIT experimental group of Pablo Jarillo-Herrero and co- workers observed superconductivity and correlated insulating states for partial fillings of the flat bands in twisted bilayer graphene (TBG) at so called magic angle [1, 2]. The experimental results in TBG samples with superconductivity and insulating states were soon confirmed by subsequent works, and many other independent groups [3-6]. Additionally, an emergent ferromagnetism near three-quarters filling of the conduction moiré band in TBG aligned with hBN has been observed [7], with a giant zero-field anomalous Hall signal and magnetohysteresis. TBG is free of atomic magnetic moments and the origin of ferromagnetism is due to correlated Chern insulator, with the anomalous Hall (AH) effect arising intrinsically from Berry curvature in the band structure. In parallel to research on TBG, twisted transition metal dichalcogenides bilayers attract prominent attention due to their potential for being new quantum simulators [8]. Unlike MATBG, in twisted TMD bilayers, moiré flat bands can be formed for a wide range of twist angles, making these systems rather insensitive to twist angles and twist-angle disorder (especially for twisted

TMD heterobilayers). Moreover, moiré TMDs superlattices exhibit peculiar optical properties and host long-lived excitons that can be electrically manipulated. Twisted TMDs provide a tunable platform to manbody Hamiltonians on a triangular or a honeycomb lattice, and in an intermediate regime, and may answer the fundamental question of whether unconventional superconductivity can emerge in a Hubbard model. Many exotic phenomena have already been observed or are predicted to emerge in these moiré materials: Mott insulators, superconductivity, Wigner crystals and charge density wave states or Chern Insulators [9, 10]. Our goal in this project is to determine and describe properties of variety of twisted heterostructures, that depends on a type of materials, twist angles and other tunable parameters. We will mainly focus on many-body effects in TBG and heterostructures from twisted transition metal dichalcogenides (TMDs). We will analyze ground and excited states properties as a function of doping for partially filled flat bands in TBG within a realistic model that includes electron-hole asymmetry, screening and alignment with hBN substrate. Combining different twisted TMDs, we will design Hubbard-like quantum simulators and determine their electronic properties by creating appropriate many-body phase diagrams. In order to do this, we will use/develop such methods as exact diagonalization, density matrix renormalization group (DMRG), Heisenberg model, Hubbard model, combined with single particle momentum space continuum model and tight-binding approach. The project will be conducted in strong collaboration with NCN OPUS project " Twistronics - research on new quantum simulators". Therefore, apart from the doctoral school's regular salary, the Ph.D. candidate will be eligible to apply for an additional project-related scholarship.

1.3. Work plan

i) literature review in the field of moiré superlattices
ii) development of theoretical models aiming for the description of a broad family of moiré materials
iii) Implementation of theoretical models as computer programs
iv) quantum simulations: calculations of electronic and magnetic properties of various moiré superlattice systems
v) analysis of results
vi) writing scientific papers and PhD thesis; auxiliary calculations

1.4. Literature *(max. 10 listed, as a suggestion for a PhD candidate)*

[1] Y. Cao et al. Nature (London) **556**, 43 (2018).
[2] Y. Cao et al. Nature (London) **556**, 80 (2018).
[4] M. Yankowitz et al. Science **363**, 11059 (2019).
[5] X. Lu et al. Nature **574**, 656 (2019).
[6] D. Wong et al. Nature **582**, 198202 (2020).
[7] A. L. Sharpe et al. Science 365, 605-608 (2019),
[8] F. Wu et al. Phys. Rev. Lett. **121**, 026402 (2018).
[9] Y. Tang et al. Nature **19**, 353 (2020).
[10] D. M. Kennes et al. Nat. Phys. **17**, 155 (2021).

1.5. Required initial knowledge and skills of the PhD candidate

i) fundamental knowledge about quantum physics.
ii) basic experience in many-body quantum mechanical calculations
iii) skills in computer programming (C,python or Fortran)
iv) commitment and good motivation for work in science!
v) MSc degree in physics or related discipline
vi) ability to read scientific papers in English

1.6. Expected development of the PhD candidate's knowledge and skills

i) expert knowledge in the field of quantum many-body physics
ii) ability to write scientific papers in English
iii) ability to present results of own research in a professional manner
iv) teamwork skills
v) experience in high-performance computation