TT 61: Focus Session: Correlations in Moiré Quantum Matter II

Time: Thursday 17:45–19:00 Location: HSZ 201

TT 61.1 Thu 17:45 HSZ 201

Magnetism and metallicity in Moiré transition metal dichalcogenides — •Patrick Tscheppe[1], Jiawei Zang[2], Marcel Klett[1], Seher Karakuzu[3], Thomas Maier[4], Michel Ferrero[5,6], Andrew Millis[2,3], and Thomas Schäfer[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Department of Physics, Columbia University, 538 West 120th Street, New York, New York 10027, USA — [3]Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, New York 10010, USA — [4]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6164, USA — [5]CPHT, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France — [6]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The Moiré transition metal dichalcogenide homobilayer WSe_2 has recently been observed both to undergo continuous Mott transitions and to display quantum critical behavior, while also allowing for high tunability of its electronic parameters. At the same time, the effective low-energy physics of WSe_2 is believed to be adequately described by a simple one-band Hubbard model. We study the rich interplay between perfect nesting and dynamical as well as non-local correlations in this model using the cellular dynamical mean-field theory (CDMFT) in conjunction with the dynamical cluster approximation (DCA). In this way we elucidate the nature of both interaction and magnetic field-driven metal-insulator crossovers, previously observed in experiments.

TT 61.2 Thu 18:00 HSZ 201

Switching between Mott-Hubbard and Hund physics in Moiré quantum simulators — •Siheon Ryee and Tim Wehling — I. Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany

Mott-Hubbard and Hund electron correlations have been realized thus far in separate classes of materials. In this talk, we show that a single Moiré homobilayer encompasses both kinds of physics in a controllable manner. We develop a microscopic multiband model which we solve by dynamical mean-field theory to nonperturbatively address the local many-body correlations. We demonstrate how tuning with twist angle, dielectric screening, and hole density allows to switch between Mott-Hubbard and Hund correlated states in twisted WSe_2 bilayer. The underlying mechanism bases on controlling Coulomb-interaction-driven orbital polarization and energetics of concomitant local singlet and triplet spin configurations. From comparison to recent experimental transport data, we find signatures of a filling-controlled transition from a triplet charge-transfer insulator to a Hund-Mott metal. Our finding establishes twisted transition metal dichalcogenides as a tunable platform for exotic phases of quantum matter emerging from large local spin moments.

TT 61.3 Thu 18:15 HSZ 201

Tunable topological order of pseudo spins in semiconductor heterostructures — Clemens Kuhlenkamp[1,2,3], •Wilhelm Kadow[1,2], Atac Imamoglu[3], and Michael Knap[1,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, D-80799 München, Germany — [3]Institute for Quantum Electronics, ETH Zürich, CH-8093 Zürich, Switzerland

We propose a novel platform to realize highly-tunable, frustrated Hubbard physics with topological order in multi-layer Moiré structures. Identifying a layer degree of freedom as a pseudo spin, allows us to retain SU(2) symmetry, while controlling ring exchange processes and concurrently quenching the kinetic energy by large external magnetic fields. This way, a broad class of interacting Hofstadter states and their transitions can be studied. Remarkably, in the limit of strong interactions the system becomes Mott insulating and we find exceptionally stable spin liquid phases which are induced by the magnetic field. As the magnetic flux can be easily tuned in Moiré systems, our approach provides a promising route towards the experimental realization and control of topologically ordered phases of matter. We also discuss how layer pseudo-spin can be probed in near-term experiments.

TT 61.4 Thu 18:30 HSZ 201

Nontrivial quantum geometry of multiband systems and implications for flat bands — •Johannes Mitscherling — Department of Physics, University of California, Berkeley, California 94720, USA

Studying the geometry of wave function manifolds helps us to identify and understand phenomena whose descriptions are not captured by the sole knowledge of the energy dispersion. A prominent example of recent interest is the distance between wave functions captured by the quantum metric. Flat-band systems are promising candidates for novel fascinating quantum metric effects since well-known contributions to observables that depend on the slope or curvature of the dispersion vanish. For instance, the dominant contribution to the superfluid stiffness and the dc electrical conductivity is proportional to the integrated quantum metric for flat bands. In this talk, I will address the role of band degeneracy in these quantum metric effects. I will use the developed framework for dc electrical conductivity [PRB 105, 085154 (2022), PRB 106, 165133 (2022)] to contrast nondegenerate and degenerate band manifolds. We will explore the common mathematical description in terms of Grassmannian manifolds and its concrete implications, such as lower bounds and the nonadditivity of the quantum metric. I close by illustrating how these concepts can be directly extended to other observables.

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TT 61.5 Thu 18:45 HSZ 201

Magnetism in twisted bilayer graphene with heterostrain — Ahmed Missaoui[1], Florie Mesple[2], Javad Vahedi[3], Andreas Honecker[1], Vincent Renard[2], and •Guy Trambly de Laissardière[1] — [1]Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, Cergy-Pontoise, France — [2]Université Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, Grenoble, France — [3]Jacobs University, School of Engineering and Science, Bremen, Germany

The discovery of correlated insulators and superconductivity due to flat bands in twisted bilayer graphene (TBG) at so-called “magic angles” has stimulated the study of their magnetic properties [1]. Furthermore, it is now well established that heterostrain, which is generally present in the samples, is a key parameter in understanding the actual shape of the flat bands [2]. Here, we present a theoretical study of magnetism in magic-angle TBG combining a Hubbard model and the mean-filed approach including non-collinear magnetic terms. We show how heterostrain strongly modifies the magnetization and the local order of magnetic state for realistic Coulomb interaction values.

[1] J. Vahedi *et al.*, SciPost Phys. **11**, 083 (2021) and references therein
[2] L. Huder *et al.*, Phys. Rev. Lett. **120**, 156405 (2018);
F. Mesple *et al.*, Phys. Rev. Lett. **127**, 126405 (2021)