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M2 Internship subject : **Which Integer fillings for Mott Physics?**

Description and expected results:

Mott insulating states, in which electronic conduction is absent despite band theory predicting the system to be a metal, are routinely found in nature - e.g. in transition-metal oxides -, and are caused by electronic correlations due to the Coulomb electron-electron repulsion.

The metallic state can be restored by chemical doping changing the carrier density, which is thus one of the main knobs tuning the physics in these systems, and in general defining the correlation strength.

The insulating Mott states (and the consequent strongly correlated metals obtained by doping them) happen when the electron density is commensurate¹², i.e. when there is an integer number of electrons per unit cell of the crystalline lattice, which naturally occurs in stoichiometric materials. The charge density is then spread between the transition metal atoms, bearing the d-orbitals responsible for the strong correlations, and the ligands that bind them.

In other systems like the heavy-fermions (and by some indications magic-angle twisted-bilayer graphene or MATBG³), however, the minimal conductive state - which can in some cases be thought as an “frustrated” Mott transition - is expected when the partial filling of the most correlated orbitals, rather than the total filling, is integer.

For both situations however the simplest model - including both a correlated and an uncorrelated orbital per unit cell - is a periodic Anderson model (PAM), implying that one should be able to bridge between these two scenarios within the parameter space of this model.

In this project, through the DMFT analysis of PAM and its variants, we aim at clarifying under which conditions the total integer filling or the partial integer filling respectively favor the maximally correlated state.

The investigation will subsequently be generalized to include multiple correlated and uncorrelated orbitals, and in general extended to more realistic, DFT-derived, models for transition-metal oxides, f-electron metals and MATBG.

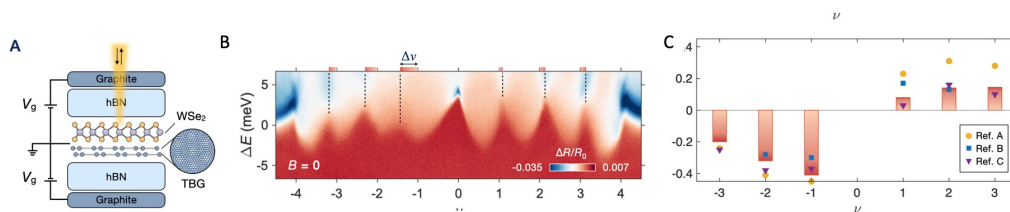


Figure 1, adapted from Ref.3. A. Schematic illustration of the device structure and optical measurement. B. Doping dependence of the reflectance contrast spectra of the device. The sawtooth feature in the 2s state originates from the nearly periodic changes in the electronic compressibility of TBG. C. Deviation Δv of the compressibility minima (indicated by dashed lines) from nearby integer fillings.

¹ A. Georges *et al.*, “Superconductivity in the two-band Hubbard model in infinite dimensions”, Z. Phys. B Condens. Matter. **92**, 313 (1993).

² A. Amaricci *et al.*, “Mott transitions with partially filled correlated orbitals”, EPL **118**, 17004 (2017).

³ Q. Hu *et al.*, “Link between cascade transitions and correlated Chern insulators in magic-angle twisted bilayer graphene”, arXiv:2406.08734 (2025).