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Resolving the VO_2 controversy: Mott mechanism dominates the insulator-to-metal transition

V Dobrosavljevic
Florida State University, USA

We consider a minimal model to investigate the metal-insulator transition in VO_2. We adopt a Hubbard model with two orbital per unit cell, which captures the competition between Mott and singlet-dimer localization. We solve the model within Dynamical Mean Field Theory, characterizing in detail the metal-insulator transition and finding new features in the electronic states. We compare our results with available experimental data obtaining good agreement in the relevant model parameter range. Crucially, we can account for puzzling optical conductivity data obtained within the hysteresis region, which we associate to a novel metallic state characterized by a split heavy quasiparticle band. Our results show that the thermal-driven insulator-to-metal transition in VO_2 is compatible with a Mott electronic mechanism, providing fresh insight to a long-standing "chicken-and-egg" debate and calling for further research of "Mottronics" applications of this system. Notably, we find Hubbard bands of a mixed character with coherent and incoherent excitations. We argue that this state is relevant for VO_2 and its signatures may be observed in spectroscopic studies, and possibly through pump-probe experiments.

vlad@magnet.fsu.edu