Magnetic fluctuations in strongly correlated systems: from toy models to realistic materials simulations

Maria Chatzieleftheriou
Institute for Theoretical Physics, Goethe University Frankfurt, Germany

Abstract: Strongly correlated electronic systems exhibit intriguing properties and highly complex phase diagrams, including metal-to-insulator transitions, magnetic/charge orderings and the field's holy grail: high temperature superconductivity. Their theoretical description is very challenging and various many-body methods have been developed to this direction. I will present results using state-of-the-art numerical techniques that allow for an accurate description of both strong local electronic correlations and spatial fluctuations. I will discuss the application of this approach on the study of a simple model, relevant for a series of materials, where we have analyzed the interplay of Mott physics and magnetic fluctuations. We have identified the Slater and Heisenberg regimes in the phase diagram, which are separated by a crossover region of competing spatial and local electronic correlations. This bridging of the two limits (the spin-fluctuation dominated Slater regime at weak coupling and the Mott insulator at strong-coupling) had been a key missing ingredient to our understanding of metal-insulator transitions in real materials. I will, moreover, present results of a recent work on the perovskite Sr_2RuO_4 compound, where we have performed realistic calculations and have accurately reproduced the experimentally estimated magnetic susceptibility, resolving a long-standing discrepancy, in the community, between theory and experiment.