Non-local Correlations in Dynamical Mean Field Theory (DMFT) calculations for realistic materials

Silke BIERMANN
Ecole Polytechnique
Centre de Physique Theorique
Route de Saclay 48
91128 Palaiseau Cedex, France

Abstract

Assessing excited states properties of materials with strong electronic Coulomb correlations is a challenge to computational solid state physics. Dynamical mean field techniques, in conjunction with electronic structure methods, have led to tremendous progress over the last years.

The basic assumption of DMFT is that electronic correlations can be captured by a local (i.e. k-independent) many-body self energy. In this talk, we present examples of materials where one needs to go beyond this paradigm: the description of spectral properties of Sr2IrO4 is significantly improved when including inter-atomic self-energies, reflecting strong antiferromagnetic fluctuations between Ir atoms present in this compound.

We show calculated spectral functions for pure and doped Sr2IrO4, in the paramagnetic and antiferromagnetic phases, finding excellent agreement with experimental data.

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