Strong-coupling formula of spin and orbital susceptibilities in the dynamical mean-field theory

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Abstract:

Dynamical mean-field theory (DMFT) is a method which is extensively employed in investigations of strongly correlated systems [1]. Applications of the DMFT have further expanded from models to materials by combining first-principles calculations within the density functional theory (DFT+DMFT) [2].

We are trying to perform susceptibility calculations in the DFT+DMFT approach, aiming at prediction of phase transitions in realistic materials. There are, however, still a pile of issues to be resolved, in particular, in multiorbital systems. Recently, we have derived a simple formula for the momentum-dependent susceptibilities in the DMFT [3]. This formula correctly captures the strong-coupling physics, namely, the kinetic exchange mechanism in the Hubbard model and the RKKY interaction in the periodic Anderson model. Thus, simpler evaluations of spin, orbital, and multipole susceptibilities become possible within DFT+DMFT framework.

In this talk, the main idea and details of the new formula will be presented with some demonstrative results.

References:

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