Electrodynamics of correlated electron: the optical conductivity as a probe for many body effects

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Phenomena that are connected to quantum mechanics, such as magnetism, transport, and the effect of impurity atoms and disorder, and their relation to material design and energy needs are important for almost every branch of the industry. Density functional theory (DFT) was successful at making accurate predictions for many materials, in particular compounds which have a metallic behaviour.

However, one bottleneck of DFT is that it fails at describing well some of the compounds where strong correlations are present, in particular because the theory has to capture both the band-like character of the uncorrelated part of the compound and the Mott-like features emerging from the local strongly correlated centres.

A recent progress has been made in this direction by the dynamical mean-field theory (DMFT), that allows describing the two limits (metal and insulator) in a remarkable precise way when combined with DFT.

We review here how DFT+DMFT can be used to investigate intermediate energy properties of the copper oxides, by comparing theoretical predictions of the optical spectra with experimental data.

In particular, we identify coherent and incoherent spectral features that result from doping a charge-transfer insulator, namely quasiparticles, Zhang-Rice singlet band, and the upper and lower Hubbard bands. We investigate the asymmetry between particle and hole doping. We discuss how the doping and temperature dependence of the optical spectral weight can be used to evaluate the strength of the correlations in hole and electron doped materials, and discriminate between Mott insulators and Slater insulators.

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