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Theoretical description of photo-doping in Mott and charge-transfer insulators

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Many aspects of photo-excited insulator-to-metal transitions in Mott and charge-transfer systems are theoretically not well understood: How is the photo-doped state related to a chemically doped state? On what timescale do we expect the formation of quasiparticles? To describe the electronic dynamics of Mott insulators, we have used nonequilibrium dynamical mean-field theory (DMFT) in combination with Quantum Monte Carlo and various weak and strong-coupling [1] techniques. In the talk, I will briefly present the current status of this approach and of related cluster approaches for nonequilibrium. I will then discuss results for the photo-doping in the Hubbard model, and in a in a p-d model for charge-transfer insulators. When the onsite Coulomb repulsion U is much larger than the hopping, rapid thermalization of the pump-excited Mott insulator is inhibited by the energetic stabilization of doublon-hole pairs [2], and various types of non-thermal states can arise. Immediately after the excitation process, the system of doublons and holes is too hot to form quasiparticle states, but coupling to a heat-bath of phonons can drive the system into a metallic state with well developed doublon and hole bands. Close to the metal-insulator transition, on the other hand, when U is of the order as the hopping, doublons and holes rapidly thermalize due to the electron-electron interaction, which makes the system a bad metal rather than a Fermi liquid.

[1] M. Eckstein and Ph. Werner, Phys. Rev. B **82**, 115115 (2010).
[2] M. Eckstein and Ph. Werner, Phys. Rev. B **84**, 035122 (2011).