Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ultrafast Response of the Hubbard Model: Non-adiabatic TDDFT+DMFT versus Non-equilibrium DMFT Solution[1] SHREE RAM ACHARYA, University of Central Florida, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics,University of Central Florida — We study the ultrafast response of electrons in the one-band Hubbard model to an external laser-pulse perturbation by using the Non-adiabatic Time-Dependent Density Functional Theory + Dynamical Mean-Field Theory (TDDFT+DMFT) approach. The corresponding exchange-correlation kernel (XC) is obtained from the DMFT charge susceptibility by using the Quantum Monte Carlo solver for the impurity problem. Detailed analysis of the time-dependent excited charge density, the Fermi distribution function, and the spatially nonhomogeneous response (metallic domain growth), is performed for different values for the carrier density and local Coulomb repulsion. We compare the results with the corresponding non-equilibrium DMFT solutions, and demonstrate that non-adiabaticity (frequency-dependence) of the XC kernel is important in order to reproduce the non-equilibrium DMFT solution. Also, from the numerical results for the charge susceptibility, we obtain an approximate analytical expression for the XC kernel. Using this kernel, we reveal possible types of "elementary" excitations and the dynamics of metallic domain growth in the case of the one-band Hubbard model. Possible generalization of the approach to the multi-orbital case is discussed.

[1]Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

Shree Ram Acharya
Department of Physics,University of Central Florida

Date submitted: 06 Nov 2015 Electronic form version 1.4