Abstract Submitted for the MAR15 Meeting of The American Physical Society

Non-adiabatic exchangecorrelation kernel for the non-equilibrium response of three-dimensional Hubbard model¹ SHREE RAM ACHARYA, NISHA BARAL, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Univ of Central Florida, Orlando, FL, 32816 — We apply Dynamical Mean-Field Theory (DMFT) to calculate the non-adiabatic (frequency-dependent) exchange-correlation kernel for the three-dimensional Hubbard model. We analyze the dependence of the kernel on the electron doping, local Coulomb repulsion and frequency by using three different impurity solvers: Hubbard-I, Iterative Perturbation Theory (IPT) and Continuous-Time Quantum Monte Carlo (CT-QMC). From the calculated data, we obtain approximate analytical expressions for the kernel. We apply the exact numerical and analytical kernels to study the non-equilibrium response of the system for applied ultrafast laser pulse. We demonstrate that the non-adiabaticity of the kernel plays an important role in the system response; in particular, leading to new excited-states involved in the system dynamics.

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

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Date submitted: 14 Nov 2014

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