Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Time-Dependent Spin-Density Functional Theory for strongly correlated systems[1] VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, FL — We present a formulation of the basic principles for a time-dependent spin-density functional theory (TDSDFT) capable of describing the main properties of strongly correlated systems. Electron-electron correlations are contained in the correlation part of the exchange-correlation (XC) kernel, which we construct using some exact results for the Hubbard model of strongly correlated electrons. The principal feature of the theory is nonadiabaticity of the XC kernel, which corresponds to a local time-resolved (oscillating in time) electron-electron interaction. As in dynamical mean-field theory, in TDSDFT such interaction defines the main properties of correlated systems, including satellite Hubbard peaks in the electronic spectrum. We demonstrate that the corresponding nonadiabatic XC kernel reproduces main features of the spectrum of the Hubbard dimer and infinite-dimensional Hubbard model, some of which are impossible to obtain within the adiabatic approach. We test the theory by applying it to several strongly correlated materials, including calculation of nonequilibrium response of these systems.

[1]Work supported in part by DOE Grant DE-FG02-07ER46354.

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Date submitted: 19 Nov 2012 Electronic form version 1.4