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A non-adiabatic exchange-correlation potential for strongly-correlated materials: local impurity approximation and beyond[1]

VOLODYMYR TURKOWSKI, SHREE RAM ACHARYA, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We formulate a non-adiabatic Time-Dependent Density-Functional Theory (TDDFT) for materials with strong local (on-site) electron-electron interactions. In this approach, the TDDFT exchange-correlation (XC) potential is derived from the expression for the single electron local-in-space self-energy obtained from the many-body Dynamical Mean-Field Theory (DMFT) solution for an effective Hubbard model (Sham-Schluter equation). We attest to the validity of the formalism through good agreement of our TDDFT results with the nonequilibrium DMFT solution for the ultrafast excited state charge dynamics of the Hubbard model for a system perturbed by a short laser pulse. To include the effects of spatial nonlocality in the XC potential, we propose a generalization of the formalism by including a momentum-dependent correction to the DMFT electron self-energy (the dynamical vertex approximation). We apply the approach to analyze the ultrafast breakdown of the insulating phase in VO2 and show that the TDDFT results are also in a good agreement with available experimental data. The developed approach can be used to study the ultrafast response of complex strongly correlated materials, a task that current many-body approaches fail to address fully because of their inherent computational demands.

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