

Abstract Submitted
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Real-time dynamics of Hubbard-type model systems via a combination of the Kadanoff-Baym formalism with adiabatic TDDFT HOPJAN MIROSLAV, Lund University, DANIEL KARLSSON, University of Jyväskylä, SIMON YDMAN, CLAUDIO VERDOZZI, CARL-OLOF ALMBLADH, Lund University — We propose a description of nonequilibrium systems via a simple protocol that combines DFT-exchange-correlation potentials with self-energies of many-body perturbation theory. The approach, aimed to avoid double counting of interactions, is tested against exact results in Hubbard-type systems, with respect to interaction strength, perturbation speed/inhomogeneity, and system dimensionality/size. In many regimes, we observe good agreement with the exact results, and an improvement over the pure adiabatic local TDDFT or the pure Second-Born NEGF approximations. We also address the reasons behind the residual discrepancies, and briefly discuss possible directions for future work.

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