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Modeling long-range time-resolved charge-transfer within TDDFT: Insights from a 2-site lattice model[1] JOHANNA FUKS, NEEPA MAITRA, Hunter College and CUNY Graduate Center — It has been shown that approximate adiabatic TDDFT functionals dramatically fail to reproduce time-resolved long-range charge-transfer dynamics (LR-CTD) [1]. In order to decouple the impact of the adiabatic approximation and the choice of ground state (gs) functional it would be instructive to propagate using the adiabatically-exact (adia-ex) functional. Numerically this involves an iterative process at each time-step to find the gs potential for a given density, which converges badly for CTD due to regions of low density. To circumvent this, we use as model system an asymmetric 2-site Hubbard model with small hopping parameter, its small Hilbert space allows to perform a Levy-Lieb constrained search and find the exact gs Hartree-exchange-correlation (Hxc) functional [2]. The later develops a sharp step feature in the long-range limit (limit of small hopping parameter). Both closed-shell to closed-shell and open-shell to open-shell LR-CT are investigated. By propagating the Kohn-Sham system in the presence of the exact gs Hxc functional under a resonant laser we are able to perform, for the first time, a fully self-consistent adia-ex propagation for CTD. [1] J. I. Fuks, P Elliott, A. Rubio, N. T. Maitra, JPCLett 4, 735 - 739 (2013) [2] J. I. Fuks et al, in preparation

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