

Abstract Submitted
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The time-dependent particle-hole map: one-dimensional benchmark studies¹ YONGHUI LI, CARSTEN ULLRICH, University of Missouri – Columbia — The time-dependent particle-hole map (TD-PHM) is a computational tool for visualization and interpretation of electronic excitation processes in many-body systems, in particular for molecular systems that are used in organic photovoltaics. In practice, the TD-PHM is obtained from time-dependent Kohn-Sham calculations, which implies three types of approximations: approximation to the exchange-correlation (xc) potential, replacement of exact many-body wave function with the corresponding Kohn-Sham Slater determinant, and, for molecules, the reduction of the six-dimensional TD-PHM to a 2-dimensional object suitable for representation in real space. Here, we focus on the first two approximations, and study one-dimensional lattice systems with several electrons interacting via soft-Coulomb potentials. We carry out benchmark calculations and to assess the validity of approximate xc potentials and the replacement of the exact wave functions with Kohn-Sham Slater determinants.

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