Implementation of orbital functionals in the context of time-dependent density functional theory

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In the last decades, time-dependent density functional theory (TDDFT) has become one of the most successful methods to approach the dynamical quantum many-body problem, which describes quantum systems that are not stationary. It consists in describing all time-dependent (TD) properties of a many-body system by using the time-evolving density as the key-variable. The most common formalism to implement TDDFT uses the so called TD Kohn-Sham (KS) equations, which considers a system of noninteracting electrons subject to an effective one-body potential, including TD and interaction effects. This potential is expressed by means of external, Hartree and exchange-correlation (XC) terms. One of the challenges is the treatment of TD XC functionals which depend only implicitly on the density, that is, the so called orbital functionals of density: they must be implemented by using the time-dependent optimized effective potential (TDOEP) method, which, however, is recognized as a tremendously computational task even when dealing with few electrons systems. In this context, we propose a comparison of different strategies of circumventing or avoiding TDOEP. Specifically, we consider three approximations to TDOEP (TDKLI, TDSlater and TDGAM), as well as, two alternatives to it (TDGSSC and TDLSSC), all of them applied to one-dimensional (1D) systems with an explicit TD dependence in the external potential. Precisely, we shall consider TDKLI – known as the most accurate approximation to TDOEP – as our reference data. As orbital functional, we use the Perdew-Zunger self-interaction correction (PZSIC) applied to an 1D local-density approximation.