

Abstract Submitted
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Exact Time-Dependent Kohn-Sham Potential for an Interacting Few-Body System RUDOLPH J. MAGYAR, Sandia National Laboratories — Time-dependent density functional theory enables practical simulations of the dynamic many-electron systems, but one of the biggest obstacles to reliable application is the quality of the approximate potential. It is often difficult to determine whether ever-more sophisticated approximations properly include new physics, as there exist few benchmark exact potentials. Towards this ends, we have developed and tested a scheme to extract the exact (non-adiabatic) time-dependent Kohn-Sham potential for few body systems. We will present some examples on 1D model systems. The approach is general and can be used to back engineer high-level quantum mechanical simulations to gain insight into TDDFT on a broad scale. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of the Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Rudolph J. Magyar
Sandia National Laboratories

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