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Numerical Density-to-Potential Inversions in Time-dependent Density Functional Theory DANIEL JENSEN, Purdue University, JEAN PIERRE INCHAUSTEGUI, Federico Villarreal National University, ADAM WASSERMAN, Purdue University — Time-dependent Density Functional Theory (TDDFT) is a formally exact method for solving the quantum many-body problem. In Kohn-Sham TDDFT, a fictitious noninteracting system is defined that exactly reproduces the time-dependent density of the interacting system. The potential that determines this noninteracting system (the time-dependent Kohn-Sham potential) has been proven to exist under certain restrictions, but finding the exact Kohn-Sham potential for a given density remains challenging. We show that this ill-posed inverse problem requires some form of regularization to produce realistic Kohn-Sham potentials. We explore various forms of regularization and illustrate how they work on simple one-dimensional model systems. We also show how our method can be applied to problems with both particle-in-a-box and periodic boundary conditions subject to oscillating electric fields.

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