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Time-dependent density functional theory for open quantum systems using unitary dynamics ALAN ASPURU-GUZIK, Department of Chemistry and Chemical Biology — We extend the Runge-Gross theorem for a very general class of Markovian and non-Markovian open quantum systems under weak assumptions about the nature of the bath and its coupling to the system. We show that for Kohn-Sham (KS) Time-Dependent Density Functional Theory, it is possible to rigorously include the effects of the environment within a bath functional in the KS potential, thus placing the interactions between the particles of the system and the coupling to the environment on the same footing. A Markovian bath functional inspired by the theory of nonlinear Schrodinger equations is suggested, which can be readily implemented in currently existing real-time codes. Finally, calculations on a helium model system are presented.

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