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Time-local equation for exact time-dependent optimized effective potential in time-dependent density functional theory[1] SHENG-LUN LIAO, National Taiwan University, TAK-SAN HO, HERSCHEL RABITZ, Princeton University, SHIH-I CHU, University of Kansas — Solving and analyzing the exact time-dependent optimized effective potential (TDOEP) integral equation has been a longstanding challenge due to its highly nonlinear and nonlocal nature. To meet the challenge, we derive an exact time-local TDOEP equation that admits a unique real-time solution in terms of time-dependent Kohn-Sham orbitals and effective memory orbitals. For illustration, the dipole evolution dynamics of a one-dimension-model chain of hydrogen atoms is numerically evaluated and examined to demonstrate the utility of the proposed time-local formulation. Importantly, it is shown that the zero-force theorem, violated by the time-dependent Krieger-Li-Iafrate approximation, is fulfilled in the current TDOEP framework.

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Shih-I Chu
University of Kansas

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