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Alternative time-dependent optimized effective potential[1] VLADIMIR NAZAROV, Research Center for Applied Sciences, Academia Sinica, Taipei 11529, Taiwan — The OEP is known as a single-particle potential minimizing the expectation value of a many-body Hamiltonian on the set of eigen-functions of a single-particle Hamiltonian [1]. The time-dependent (TD) OEP can be constructed with the TD quantum stationary-action principle [2]. Very useful conceptually in DFT and TDDFT, both OEPs are not practicable due to the complexity of their implementations. Here we report a TDOEP by minimizing the difference of LHS and RHS of the TD Schrödinger equation [3]. If the orbitals are varied, then the TD Hartree-Fock equations are reproduced. Similarly, we now find the OEP. New OMP does not involve the inversion of the density-response function χ_s, which greatly facilitates implementations. Accordingly, the exchange-correlation kernel f_{xc} involves of χ_s^{-1} only, not its quadratic counterpart. To show the power of this method, we work out the $f_{xc}^h(q,\omega)$ of the homogeneous electron gas to be used with the nearly-free electrons theory, where f_{xc}^h is the main input [4].

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