Abstract Submitted
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Relaxation and dissipation in time-dependent current-density functional theory[1] ROBERTO D'AGOSTA, GIOVANNI VIGNALE, University of Missouri — In a typical relaxation problem a many-particle system evolves from an initial excited state under the action of its own hamiltonian plus a "thermal bath", until equilibrium (or the ground-state at $T = 0$) is reached. Due to the presence of the thermal bath the time evolution of the system is not unitary, and an initially pure state will evolve into a statistical mixture of states. Here we show that the time-dependent current density functional theory[1] allows a hamiltonian description of the relaxation process, whereby the quantum state of the system undergoes a unitary time evolution without becoming entangled with a thermal bath. The essential feature that causes the system to eventually settle into a stationary state of the ground-state Kohn-Sham hamiltonian is the presence of an effective electric field, which is determined by the instantaneous values of the current and the density. Our theory is consistent with recent numerical results by Wijewardane and Ullrich[2].
1. G. Vignale, C. A. Ullrich, and S. Conti, PRL **79**, 4878 (1997)
2. H. O. Wijewardane and C. A. Ullrich, cond-mat/0411157

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