A physical interpretation of the Kohn-Sham energy in time-dependent current-density functional theory ROBERTO D'AGOSTA, Department of Physics, University of California - San Diego, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri - Columbia — It is well known that in static density functional theory the Kohn-Sham energy plays a fundamental role because it gives, by construction, the ground state energy of the system under study. In time-dependent density functional theory, it is not possible to attach to the Kohn-Sham energy the same physical interpretation. For example we know that for an isolated system the Kohn-Sham energy can be "dissipated" while the total energy of the real system is conserved.[1] However, the Kohn-Sham energy can be given a new physical interpretation as the maximum work that can be extracted from the system and it is related to the production of entropy during the time evolution of the system.[1] Project supported by NFS Grant No. DMR-0313681

[1]R. D'Agosta and G. Vignale, accepted by Phys. Rev. Lett., cond-mat/0508175

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