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Meta-GGA-based adiabatic time-dependent density-functional theory[1] VLADIMIR NAZAROV, Research Center for Applied Sciences, Academia Sinica, GIOVANNI VIGNALE, University of Missouri-Columbia — The local-density approximation (LDA) to the ground-state density functional theory (DFT) is well known to allow for a generalization to the time-dependent case [1]. The assumption of the adiabaticity of the process greatly simplifies the theory. The further extension of the time-dependent DFT (TDDFT) to the generalized gradient approximation (GGA) is trivial. Here we address lifting the adiabatic TDDFT to the third rung of the "Jacobs ladder" [2] : We work out the kinetic energy density dependent (meta-GGA) TDDFT formalism. The new theory possesses remarkable properties not present in LDA and GGA: (i) It is non-local with respect to the particle density; (ii) In the case of bulk semiconductors, it supports the $1/q^2$ singularity of the exchange-correlation kernel, where q is the wave-vector, the latter being important to reproduce the excitonic effect. We also present illustrative calculations of the optical absorption in semiconductors [3].

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