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Dynamical exchange-correlation potentials beyond the local density approximation[1] JIANMIN TAO, GIOVANNI VIGNALE, University of Missouri — Approximations for the static exchange-correlation (xc) potential of density functional theory (DFT) have reached a high level of sophistication. By contrast, time-dependent xc potentials are still being treated in a local (although velocity-dependent) approximation [G. Vignale, C. A. Ullrich and S. Conti, PRL **79**, 4879 (1997)]. Unfortunately, one of the assumptions upon which the dynamical local approximation is based appears to break down in the important case of d.c. transport. Here we propose a new approximation scheme, which should allow a more accurate treatment of molecular transport problems. As a first step, we separate the exact adiabatic xc potential, which has the same form as in the static theory and can be treated by a generalized gradient approximation (GGA) or a meta-GGA. In the second step, we express the high-frequency limit of the xc stress tensor (whose divergence gives the xc force density) in terms of the exact static xc energy functional. Finally, we develop a perturbative scheme for the calculation of the frequency dependence of the xc stress tensor in terms of the ground-state Kohn-Sham orbitals and eigenvalues.

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