

Nonlocal exchange-correlation kernel from time-dependent current density functional theory: Application to the stopping power of an electron liquid

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We develop a procedure for building the scalar exchange-correlation kernel of time-dependent density functional theory (TDDFT) from the tensorial kernel of time-dependent *current* density functional theory [1] (TDCDFT) and the Kohn-Sham current-density response function. Doing the local approximation on the kernel of TDCDFT results in a nonlocal approximation for the kernel of TDDFT, which is free of the contradictions that plague the standard local density approximation to TDDFT. As an application of the general formalism, we calculate the dynamical exchange-correlation contribution to the stopping power of an electron liquid for slow ions. The results of this calculation are found to be in considerably better agreement with experiment [2] than the results obtained from a conventional TDDFT calculation in the local density approximation [3].

[1]. G. Vignale and W. Kohn, Phys. Rev. Lett. **77**, 2037 (1996).

[2]. H. Winter, J. I. Juaristi, I. Nagy, A. Arnau, and P. M. Echenique, Phys. Rev. B **67**, 245401 (2003).

[3]. V. U. Nazarov, J. M. Pitarke, C. S. Kim, and Y. Takada, Phys. Rev. B **71**, 121106 (2005).