

Abstract Submitted
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Generator coordinates: a new road towards dynamics and excitations in DFT¹ KLAUS CAPELLE, University of Sao Paulo — The generator-coordinate method is a flexible and powerful reformulation of the variational principle. Here we show that by introducing a generator coordinate in the Kohn-Sham equation of density-functional theory, excitation energies can be obtained from ground-state density functionals. Similarly, by introducing a generator coordinate in the equations of time-dependent DFT, memory effects can be built into any existing adiabatic exchange-correlation potential. (See J. Chem. Phys. 127, p. 124101 (2007) and J. Chem. Phys. 119, p. 1285 (2003).)

¹Work done in collaboration with E. Orestes, C.A. Ullrich and A.B.F. da Silva

Klaus Capelle
University of Sao Paulo

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