Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

The Generating-Coordinate Method in Static and Time-Dependent Density Functional Theory[1] EDNILSOM ORESTES, Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo and Department of Physics and Astronomy, University of Missouri-Columbia, A. B. F. DA SILVA, Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, KLAUS CAPELLE, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, CARSTEN A. ULLRICH, Department of Physics and Astronomy, University of Missouri-Columbia — The generating-coordinate method represents a many-body wave function as a superposition of non-orthogonal Kohn-Sham Slater determinants arising from different Hamiltonians. This method provides additional variational degrees of freedom in the calculation of static and dynamical properties of electronic systems. We present results for atomic ground- and excited- state energies for various choices of generating coordinates. We then apply our variational approach to discuss a particularly challenging problem in TDDFT, the calculation of correlated double-ionization processes. We present results for single- and double-ionization probabilities of a strongly driven two-electron Hookes atom.

[1]Work supported by NSF Grant No. DMR-0553485 and Research Corporation.

Carsten A. Ullrich
Department of Physics and Astronomy, University of Missouri-Columbia

Date submitted: 29 Nov 2005 Electronic form version 1.4