Improved Polarizabilities and Dissociation in DFT: Vignale-Kohn Revisited NEEPA MAITRA, Hunter College and the City University of New York, New York, META VAN FAASSEN, Rutgers University, Piscataway, NJ — We develop a novel approach to the problem of polarizabilities and dissociation in electric fields from the static limit of the Vignale-Kohn (VK) functional. The VK response potential, extracted from the longitudinal component of the VK vector potential has ground-state properties that notably improve over VK response and over usual (semi-)local functionals. The VK density response is not the ground-state response in the corresponding field. Cases where VK density response yields poor polarizabilities, eg the H2 chain, work well in our approach. This is the first density functional method that correctly dissociates open-shell fragments in a field.

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