Density Functional with Full Exact Exchange, Balanced Nonlocality of Correlation, and Constraint Satisfaction[1] JOHN P. PERDEW, Physics, Tulane U., VIKTOR N. STAROVEROV, Chemistry, U. of Western Ontario, JIANMIN TAO, Los Alamos National Lab, GUSTAVO E. SCUSERIA, Chemistry, Rice U. — We construct a nonlocal density functional with full exact exchange, while preserving the constraint-satisfaction approach and justified error cancellations of simpler semilocal functionals. This is achieved by interpolating between different approximations suitable for two extreme regions of the electron density. In a "normal region", the exact exchange-correlation hole around an electron is semilocal because its range is reduced by correlation and because it integrates over a narrow range to -1. "Abnormal" regions, where nonlocality is unveiled, include those in which exchange can dominate correlation (one-electron, nonuniform high density, and rapidly-varying limits), and those open systems of fluctuating electron number over which the exact exchange-correlation hole integrates to a value greater than -1. Regions between these extremes are described by a local hybrid mixing exact and semilocal exchange locally.

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