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Exact Expressions for Exchange-Correlation Potentials

VIKTOR STAROVEROV, Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7

The Baerends and Staroverov groups have devised various exact expressions for the exchange-correlation potential in terms of wave-function and Kohn–Sham ingredients. We show that all these expressions can be obtained as special cases of one general approach. One particular expression derived by us involves at most the two-electron reduced density matrix and is ideally suited for practical calculations of exchange-correlation potentials from many-electron wave functions, as demonstrated by numerical examples. Interesting identities emerging from our derivation are also presented and discussed.