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Anti-Hermitian Contracted Schrödinger Equation for the Determination of Ground-state Energies and Two-electron Reduced-density-matrices without Wavefunctions[1] DAVID MAZZIOTTI — A recent advance in the theory of the contracted Schrödinger equation (CSE), in which only the anti-Hermitian part of the equation is solved, permits the direct determination of ground-state two-electron reduced density matrices (2-RDMs) that yield 95-100% of the correlation energy of atoms and molecules [Mazziotti, Phys. Rev. Lett. **97**, 143002 (2006)]. Here we discuss in detail the anti-Hermitian contracted Schrödinger equation (ACSE) and its comparison to the CSE with regard to cumulant reconstruction of RDMs, the role of Nakatsuji's theorem, and the structure of the wavefunction. The ACSE is also formulated in the Heisenberg representation and related to canonical diagonalization. The solution of the ACSE is illustrated with a variety of molecules. The computed 2-RDMs very closely satisfy known N-representability conditions.

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