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Two-electron Reduced-Density-Matrix Mechanics: With Application to Many-electron Atoms and Molecules

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In 1959 Charles Coulson popularized the challenge of computing the ground-state energy as a functional of the two-electron reduced density matrix (2-RDM) without the many-electron wavefunction. Recently, theoretical and computational advances have led to two classes of 2-RDM methods [1]: (i) the variational calculation of the 2-RDM subject to approximate N-representability conditions and (ii) the non-variational calculation of the 2-RDM from the anti-Hermitian contracted Schrödinger equation. I will develop the background for the 2-RDM methods, discuss recent theoretical and computational advances, and present some applications, including the detection of poly-radical correlation in polyaromatic acene and aryne chains, the study of protonated acetylene and malonaldehyde beyond the Born-Oppenheimer approximation, and the computation of activation energies in pericyclic reactions of open- and closed-shell molecular species.

[1] "Two-electron Reduced-Density-Matrix Mechanics with Application to Many-electron Atoms and Molecules," edited by D. A. Mazziotti, Advances in Chemical Physics Vol. 134 (Wiley, New York, 2007).