

Linear-Expansion Shooting Techniques for Accelerating Self-Consistent Field Convergence

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Based on the corrected Hohenberg-Kohn-Sham energy functional (cHKS) [1,2], we present a new method to accelerate self-consistent field (SCF) convergence by utilizing the shooting method in numerical analysis [3]. We have developed several different linear-expansion shooting techniques (LIST) by imposing different conditions [4]. Case studies show that overall our LIST methods are robust and efficient algorithms for accelerating SCF convergence. More importantly, the LIST methods outperform Pulay's DIIS [5,6] and its recent improvements, including EDIIS [7] and ADIIS [8].

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