Approximate Connected Moments for Use in Many-Body Calculations

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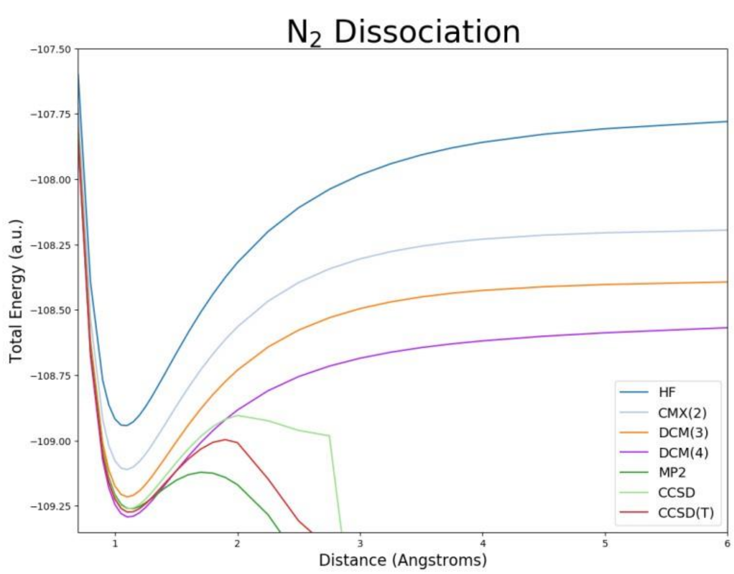
The Horn-Weinstein theorem[1] provides a route to the true ground state energy via higher-order moments of the Hamiltonian for an arbitrary reference determinant. That seminal work has spawned various many-body methods involving these values; for chemistry in particular, the connected-moment expansion [CMX(n)] with a Hartree-Fock wavefunction saw success as a non-perturbative, size-extensive, and systematically improvable approach for the calculation of the correlation energy and complimentary to many-body perturbation theory [MBPT(n)] and various infinite-order approaches. With the growing success of the latter quantum chemical methodologies, the body of literature surrounding Hamiltonian moments has waned with slight revivals through the years addressing affordability, accuracy, and alternative ansatzes to this approach. In the same vein, we investigate new possibilities in regards to connected moments. These advents focus on the creation of new approximations for connected moments as well as the evaluation schemes for their use in solving ground and excited state energies. Selectively summing linked moments with arbitrarily-high connected N-body contributions are presented and are used as intermediates in an exponential expansions of the Horn-Weinstein theorem. The procedure is compared against various quantum chemical methods to determine the efficacy of the new approach, and is shown to be tractable compared to other popular many-body methods.



1. Horn, D. & Weinstein, M. (1984) The t-expansion: A nonperturbative analytic tool for Hamiltonian systems. Phys. Rev. D 30, 1256–1270.