Cubic-scaling algorithm and self-consistent mean field for random-phase approximation with second-order screened exchange

Jonathan E. Moussa[1]

Sandia National Laboratories, Albuquerque, NM 87185, USA

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The random-phase approximation with second-order screened exchange (RPA+SOSEX) is a model of electron correlation energy with two caveats: its accuracy depends on an arbitrary choice of mean field, and it scales as $\mathcal{O}(n^5)$ operations and $\mathcal{O}(n^3)$ memory for n electrons. We derive a new algorithm to reduce its scaling to $\mathcal{O}(n^3)$ operations and $\mathcal{O}(n^2)$ memory and derive a self-consistent mean field by constructing RPA+SOSEX as an approximation to Brueckner coupled-cluster doubles (BCCD) theory. We verify the new model's accuracy on the dissociation of H_2 and verify the new algorithm's scaling on H_n rings. The revised RPA+SOSEX model is a nonempirical alternative to conventional density functional theory (DFT) with a higher cost but equivalent scaling.

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