Abstract Submitted
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Stochastic Coupled Cluster Theory ALEX J. W. THOM, Department of Chemistry, University of Cambridge, Cambridge, UK — In an extension of the Full Configuration Interaction Monte Carlo method of Alavi et al.[1], I describe a stochastic algorithm to perform Coupled Cluster Theory[2] which represents excitation amplitudes as populations discrete excitation particles (excips) in the space of excitation operators (excitors). Re-expressing the Coupled Cluster equations as the dynamics of excips in this space, we show that a simple set of rules consisting of spawning, death, and annihilation steps suffice to evolve a distribution of in the space of excitors to sample the Coupled Cluster solution and correctly evaluate its energy. These rules are extremely simple to implement and not truncation-specific and thus this method can calculate solutions to an arbitrary level of truncation. I present results of CCSDTQ calculations on the neon atom with basis sets up to cc-pV6Z as well as calculations on the uniform electron gas beyond the capability of other present methods.

[1] GH Booth, AJW Thom, A Alavi, J. Chem. Phys. (2009) 131, 054106
[2] AJW Thom, Phys. Rev. Lett. (2010) 105, 263004

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