A Stochastic Implementation of Second-order Green's Function Perturbation Theory

Determining the electronic structure of realistic materials or molecules using ab-initio systematically improvable methods is a difficult problem.   At present, many wave function and density employing formalisms have been investigated in detail yielding very robust methods to calculate energetics. However, much less is explored about Green's function type methods capable of producing spectra or thermodynamics. Of recent, the self-consistent second-order Green's Function (GF2) approach has shown consistency in accurately describing weakly and moderately strongly correlated systems; however, the computational scaling of GF2 is expensive enough to deter its easy application to periodic, or even large, molecular systems. We are developing a stochastic implementation of GF2 in order to access larger systems by systematically sampling all the second order expansion contributions and neglecting the smallest, unimportant terms. In this work, I will describe the sampling procedure, as well as show the progress in benchmarking simpler to more complex systems.