Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Many Body Density Matrix Theory[1] C.J. TYMCZAK, Texas Southern University — One fundamental limitation of quantum chemical methods is the accuracy of the approximate many-body theoretical framework. Accurate many-body formalisms for quantum chemical methods do exist, but these methods are computationally very expensive. Methods also exist that are much less computationally expensive such as Hatree-Fock, Density Functional and the Hybrid Functional theories, but at a reduced representation of the exact many-body ground state. This severely limits either the system size that can be addressed accurately, or the accuracy of the representation. What is needed is a method that represents the many-body ground states accurately, but with a low computational cost. Recently, a method for determining the response, to any order of the perturbation, within the density matrix formalism has been discovered. This method opens up the possibility of computing the variational many-body ground states to unprecedented accuracy within a simplified computational approach. We report on the theoretical development of this methodology, which we refer to as Many Body Density Matrix Theory. This theory has many significant advantages over existing methods. One, its computational cost is equivalent to Hartree-Fock or Density Functional theory. Two it is a variational upper bound to the exact many-body ground state energy. Three, like Hartree-Fock, it has no self-interaction. And four, it is size extensive.

[1]Funded by Welch Foundation Grant J-1675

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Date submitted: 14 Dec 2010 Electronic form version 1.4