Linear Scaling Properties of One- and Two-Electron Integrals, Fock Operator, and Molecular Orbitals

Alexander V. Mitin

Center for Environmental Kinetics Analysis, The Pennsylvania State University, 2217 EES Building, University Park, PA 16802

The first-principle electronic structure theory operates with such main quantities as one- and two-electron integrals, the Fock and electron density operators, and molecular orbitals. The knowledge of scaling properties of these quantities is very important for developments of efficient *ab initio* methods and programs.

Discovering the linear scaling property of density matrix by Kohn [1] has a significant impact on further theoretical and program developments. The explicit use of this property permits to develop efficient linear scaling Hartree-Fock and density functional methods and programs for *ab initio* quantum calculations of large molecules and solids. Now it is widely accepted that such methods are more suitable for calculations of large molecular systems compared to the conventional self consistent iterations introduced by Hartree [2].

A number of two-electron integrals (N_{2e}) scales formally as N^4 for a system with N basis functions. However in [3] it was analytically shown that (N_{2e}) scales as $N^2(lnN)^2$. Later, without a proof it was noted that N_{2e} scales as $N^2(lnN)$ [4]. The estimation that N_{2e} scales as $N^{2.2\text{-}2.3}$ which has been reported in [5] is now the widely accepted. However, an analysis of the procedure used in this work for obtaining an optimal power of N shows that there is a deep inconsistence between the global data fitting and counting only non-zero integrals. The global data fitting implies that two-electron integrals globally depend on molecular coordinates. But the non-zero integrals reflect just the local properties of molecular systems. Therefore the power dependence of two-electron integrals on the system size can be correctly investigated only through investigations of the local or differential properties of this dependence.

The scaling properties of one-electron integrals, the Fock operator, and molecular orbitals have not been investigated yet.

In these connections the scaling properties of one- and two-electron integrals, the Fock operator, and molecular orbitals have been investigated in the present study. In has been shown that all these quantities possess the linear scaling property with respect to the number of basis functions for large systems [6].

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