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Multiresolution Quantum Chemistry in Multiwavelet Bases:

Analytic gradient and linear response theory in Hartree-Fock/Kohn-Sham method

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Abstract

A new numerical computation approach for molecular electronic structure theory is presented employing the multiresolution analysis in multiwavelet bases with low-separation rank representation. Our object is to develop an alternative computational framework (including software) for electronic structure computation that is free of basis set error, scales correctly with the system size, and is based upon a firm mathematical foundation oriented toward fast computation with guaranteed accuracy.

In this presentation, we discuss the mathematical background on the multiresolution analysis, several theoretical aspects on initial application to Hartree-Fock and density functional theory, and the primitive (prototype) implementations 'MADNESS' (multiresolution adaptive numerical scientific simulation).

The illustrative results will be provided with respect to the analytic gradient method using the Hellmann-Feynman theorem and the excitation calculation via linear response theory in Hartree-Fock and density functional theory.

Keywords: multiresolution analysis, multiwavelets, low-separation rank, O(*N*) computation, Hartree-Fock, density functional theory, analytic gradient, Hellmann-Feynman theorem, linear response theory, time-dependent Hartree-Fock / density functional theory (TD-HF/DFT)

Multiresolution Quantum Chemistry in Multiwavelet Bases: Hartree-Fock/Kohn-Sham 法の解析的微分法と励起状態計算法

要旨: Multiwavelet に基づく Multiresolution（多重解像度）解析を用いて、電子状態理論（特に分子軌道法）の新しい数値計算法と理論的アプローチを発表する。本発表では、積分演算子を活用した Hartree-Fock / Kohn-Sham-SCF 法の解法、線形応答法からの励起状態計算法、Helmann-Feynmann theorem を用いた解析的微分法、また幾つかの応用計算例を紹介する。本手法は、保証精度の内で基底関数誤差は無く、分子のサイズに対して正しく計算コストがスケーリングするように開発されている。