**Development of computer program for electronic structure calculation using Lagrange basis functions**

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**ABSTRACT**

Electronic structure calculation is one approach that can be used to study material, especially at nanoscale where quantum nature of electrons might play important role to determine material properties. Among various methods for electronic structure calculation, density functional theory (DFT) based on Kohn-Sham equations is considered to be a popular one. In the the implementation to solve Kohn-Sham equations, single-electron wave function must be represented as an expansion of basis functions or some discretization schemes. Several existing computer programs for DFT calculations, such as Quantum Espresso and Gaussian09, expand single-electron wave function using plane wave and Gaussian functions, respectively. Others, such as Octopus and GPAW use discretization based on finite-difference scheme. In this article, we report our initial effort to implement a new computer program to solve Kohn-Sham equations using expansion in Lagrange basis functions (LFs). Use of this basis set in Kohn-Sham equation results in matrix eigenproblem which is similar to matrix eigenproblem in finite difference schemes. Two methods to solve Kohn-Sham equation, namely self-consistent field iterations and direct minimization, are reported. Comparisons done with finite difference scheme implemented in Octopus for several simple systems shows that total energy convergence with respect to the number of grid points is better when using Lagrange basis functions.

**Keywords**: electronic structure, density functional theory, Kohn-Sham equations, Lagrange basis functions, finite difference scheme