Convergence study of isogeometric analysis in electronic structure calculations

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ABSTRACT

We present a study of convergence and accuracy properties of isogeometric analysis applied for electronic structure calculations [1]. A new method [2] for non-periodic electronic structures based on the density functional theory, environment-reflecting pseudopotentials and the isogeometric analysis with Bézier extraction has been developed and tested. The approach is especially suitable for calculating the total energy and its second derivatives and mainly for evaluation of atomic forces based on the Hellmann-Feynman theorem.

Within the contribution, convergence study for isogeometric analysis vs. standard finite-element approach is carried out and illustrated on sub-problems that appear in our electronic structure calculations method: the Poisson problem, the generalized eigenvalue problem and the Kohn – Sham self-consistent solution problem within density functional theory. The effect of order and continuity of spline shape function is analyzed [3]. It seems that the isogeometric analysis is an excellent tool for accurate calculations of electronic structure behavior.

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