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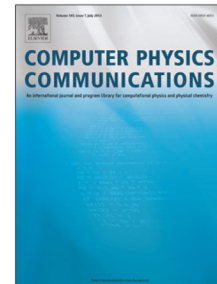
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Tensor decompositions for the bubbles and cube numerical framework

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Abstract

Canonical decomposition methods and the Tucker decomposition method have been applied to the cube part of the orbitals in the bubbles and cube framework for numerical electronic structure calculations on molecules. The iterative process of two variants of the alternating least squares method for performing canonical decomposition is found to converge rapidly to a given accuracy, whereas the accuracy is not significantly improved by continuing the iterations, implying that the studied canonical decomposition methods are not of practical use in our approach to numerical electronic structure calculations. The Tucker decomposition method of the orbitals is on the other hand found to have relative errors that are smaller than the numerical accuracy of the orbitals. The calculations also show that the reconstruction of the orbitals leads to errors that are well below the required accuracy.

Keywords: Tucker-type tensor decomposition, Electronic structure calculations, Canonical decomposition, Numerical basis functions, Lossy compression

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