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Solving coupled cluster equations using tensor train decomposition

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The achievement of high accuracy in theoretical modeling of the electronic structure of materials containing f-elements, in particular lanthanides and actinides, requires simultaneous consideration of relativistic and correlation effects. The most promising method that satisfies this requirement is the relativistic coupled cluster method (RCC), which leads to extremely resource-intensive calculations. It is possible to achieve increased capabilities and reduced computational complexity by using tensor decompositions to store data and optimize the algorithms used in modeling.

For this purpose, a detailed analysis of the efficiency of various tensor decomposition schemes (canonical [1], tensor train [2] and Tucker [3] decompositions) were carried out. Optimal algorithms were found for performing the approximate decomposition of tensors of molecular integrals and cluster amplitudes, and the computational complexity of algorithms implementing the basic operations of the working equations of the coupled cluster method was evaluated.

For the first time, the equations of the coupled cluster method for the ground state were formulated directly in terms of tensor trains, including versions of the method that take into account the contributions of triple excitations of reference functions. Also a software implementation was performed and include to the EXP-T quantum chemical package [4]. Pilot calculations using CCSD method was carried out, in which the superiority of solving the equations of the coupled cluster method in terms of tensor trains was shown.

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[3] Tucker L. R. Some mathematical notes on three-mode factor analysis // Psychometrika. 1966. V. 31, no. 3. PP. 279–311. doi: 10.1007/BF02289464.
[4] Oleynichenko A. V., Zaitsevskii A., Eliav E. Towards High Performance Relativistic Electronic Structure Modelling: The EXP-T Program Package // Supercomputing. Springer International Publishing, 2020. PP. 375–386. doi: 10.1007/978-3-030-64616-5 33.

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