Regularized Relativistic Corrections for Molecular Systems

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This research report elaborates on a newly developed methodology for obtaining regularized relativistic corrections for small molecular systems.

In the beginning, the need for highly precise theoretical results is introduced to verify experimental results. The first section is dedicated to creating a necessary theoretical framework, which the rest of the sections rely on, with the topics detailed being: the foundations of non-relativistic quantum chemistry, the variational method, explicitly correlated Gaussian functions (ECGs) and perturbative approaches. With the understanding of the necessity of FECGs, three analytically unknown matrix elements are identified as the cause of the square of the Hamiltonian operator being incalculable for molecules. The importance of this operator is highlighted, detailing its applications primarily for regularization techniques for relativistic corrections, as well as a brief discussion on exact energy lower bound calculations. After this, a solution is introduced for evaluating the incalculable matrix elements in the form of an approximation, proposed by Beylkin and Monzón [1]. The key steps of the formula's derivation are detailed, with the recounting of investigations into the choice of the parameters, as well as considerations regarding the shape of the basis functions.

The essence of this paper is focused on the integration of this approximation to evaluate the three matrix elements identified. The required derivations are detailed along with the challenges and subcases that needed to be accounted for. The resulting methodology is exceedingly robust, backed by the promising numerical computations presented. Results of regularized singular operators of relativistic corrections are showcased for the He atom and the H3+ cation. The paper concludes with a summary and outlook on ongoing and future works regarding the methodology.

[1] Beylkin G., Monzón L., *Applied and Computational Harmonic Analysis*, vol. 19, pp. 17–48, (2005)