# One-dimensional model for relativistic quantum chemistry: A first step towards the development of a relativistic DFT

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ABSTRACT

It is important to take into account the effects of special relativity in the quantum description of chemical systems with heavy elements. The relativistic effects account for gold's color, mercury's liquid state at room temperature and are responsible for the efficiency of lead-acid batteries in cars [1]. Relativistic electronic-structure computational methods have been developed in the no-pair approximation, and are now routinely applied on molecular systems. Hence, the next challenge is to go beyond the no-pair approximation by including the quantum-electrodynamics (QED) effects of virtual electron-positron pairs. Such description is needed to recover some properties, even in very simple systems, *e.g.* the Lamb shift in the Hydrogen atom.

In this work we are interested in an one-dimensional model of relativistic hydrogen-like atom using delta-potential interactions. It is motivated by the non-relativistic version of this model which leads to the same ground-state energy and radial wave function as the three-dimensional one [2]. We are using an effective QED Hamiltonian which includes the effect of the vacuum polarization, and the creation of electron-positron pairs, but does not include the photons degree of freedom [4,5,6]. In this model we are able to make accurate QED calculations [7]. Using these results we are developing a more rigorous mathematical background on which the development of a one-dimensional relativistic-DFT (RDFT) can be properly investigated. This development could be a next step towards a development of a three-dimensional RDFT taking QED effects into account.

# References

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