Some novel physical insights about the spin and spin-dependent properties

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The spin variable is one of the most used in quantum chemistry. It was postulated in 1925 to explain previous experimental results (Stern-Gerlach) and then included in the solutions of Schrödinger equation. From that time spin interactions have profound effects in chemistry.. But spin neither has any classical analog nor is well defined within the relativistic framework.

The description of the electronic behavior of heavy-atom containing molecules (atoms belonging to the 5^{th} and 6^{th} row of the periodic table) must be given within the relativistic quantum chemistry.[1] Within this regime the treatment of magnetic properties apply models and methods similar but generalized of that used within the NR regime. Polarization propagtors are also valid and in this case new physical concepts and understandings do arise.[2]

Within the relativistic framework the wave function is not any longer scalar but it has four-components and the Hamiltonian cannot be defined in an exact manner. On the other hand the spin is not a good quantum number so that one must find the way to redefine useful computational advantages and properties in which the spin is central within the NR framework. One cannot continues using singlet- and triplet-type descriptions and must apply the time-reversal symmetry.

The main spectroscopic parameters of the nuclear magnetic resonance spectroscopy, NMR, the nuclear magnetic shielding and indirect J-couplings, which are defined through singlet-type, and triplet- and singlet-type electronic mechanisms, respectively, must be redefined. Besides paramagnetic and diamagnetic contributions are unified due to they arise from a unique relativistic mechanism.[3] There are new effects that should be included in accurate calculations like QED, relativistic and nuclear-size effects.

In this seminar I will discuss about the nature of the nuclear and electron spin and then I will give some basic elements of relativistic quantum chemistry. I will define and use polarization propagators to show some interesting new insights that appears when one works within the relativistic framework.[3] I will at the end of the presentation show results of recent studies involving entanglement among pairs of LMO excitations and QED and relativistic effects.[4]

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4. L. A. Millán, C. G. Giribet and G. A. Aucar, Phys. Chem. Chem. Phys. **20**, 24832 (2018); K. Koziol, I. A. Aucar and G. A. Aucar, J. Chem. Phys. **150**, 184301 (2019).