

Relativistic polarization propagators within the path integral formalism

One of the straight ways to analyze entanglement and QED effects on response properties

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Polarization propagators are theoretical objects that were first developed within the non relativistic, NR, framework in the 1970's.[1] Their main applications were focused on response properties, like NMR spectroscopic parameters. Its generalization to the relativistic framework was uncovered in the early 1990's [2] and, after another twenty years, they were found to be nicely obtainable from the path integral formalism,[3] from which one can explain some of the previous findings common to both regimes, NR and relativistic. This new formalism opened new ways to include QED effects on response properties.

In this presentation I will show some of the new understandings that arises after deriving polarization propagators from the path integral formalism, and writing them within the relativistic framework. I will focus on the physics that underlies the atomic and molecular response properties, and a model from which one can introduce QED and Gaunt effects,[4] to get accurate theoretical values of NMR spectroscopic parameters. I will also show one of the newest findings, the likely entanglement between excitations of molecular orbitals.[5]

1. P. Jørgensen and J. Oddershede, *J. Chem. Phys.* 1972, **57**, 277; J. Oddershede, *Adv. Quant. Chem.* 1978, **11**, 257.
2. G. A. Aucar and J. Oddershede, *Int. J. Quantum Chem.* 1993, **47**, 425; G. A. Aucar, T. Saue, L. Visscher and H. J. Aa. Jensen, *J. Chem. Phys.* 1999, **110**, 6208; G. A. Aucar, A. F. Maldonado, M. D. A. Montero and T. Santa Cruz, *Int J Quantum Chem.* 2019;**119**:e25722.
3. G. A. Aucar, *Phys. Chem. Chem. Phys.* 2014, **16**, 4420.
4. K. Koziol, I. A. Aucar and G. A. Aucar, *J. Chem. Phys.* 2019, **150**, 184301.
5. L. A. Millán, C. G. Giribet and G. A. Aucar, *Phys. Chem. Chem. Phys.* 2018, **20**, 24832.