Flexible toolbox for calculation of relativistic properties with two-component densities

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Relativistic effects typically play an important role for the theoretical description of heavy-elemental compounds and in calculations of properties that depend strongly on the structure of the electronic wave function close to the nuclei, such as NMR shielding constants. For many purposes, however, it is not necessary to perform four-component relativistic calculations, but quasi-relativistic two-component methods often suffice. This applies even in case of so-called purely relativistic effects, as we have shown for molecular enhancements of a hypothetical electric dipole moment of the electron (eEDM).[1]
Nowadays, many programs are capable of two-component calculations. Nonetheless, the majority of two-component programs is restricted to conventional molecular properties, such as NMR-shielding constants or g-tensors. This is often caused by the fact that the calculation of relativistic molecular properties with one- or two-component wave function requires a proper transformation of the operators into the appropriate picture. The implementation of less conventional properties, such as parity violating energy shifts or other intriguing effects, often is done by hand and not available as an out-of-the-box feature. Thus an automated evaluation of custom one-electron properties with efficiently calculated two-component wave functions is of great use.
In this poster a general formulation of relativistic one-electron properties in terms of density functions is presented, which allows for customized definition of operators within a generic two-component property module. An implementation within a two-component zeroth order regular approximation (ZORA) framework for the use with a modified version of the Turbomole program package[2] is outlined. Within this implementation arbitrary relativistic properties can be calculated, ranging from symmetry violating properties which are of importance for different fundamental physics tests, to conventional hyperfine coupling, electric field gradients or NMR shielding tensors.

References

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[2] Ahlrichs, R., Bär, M., Häser, M., Horn, H. and Kölmel, C. *Chem. Phys. Lett.*, **1989**, *162*, 165; van Wllen, C. *J. Chem. Phys.*, **1998**, *109*, 392.