Self-consistent treatment of the frequency-independent Breit interaction in atomic structure calculations.

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The self-consistent treatment of the Breit interaction in fully numerical atomic structure calculations is extremely cumbersome due to the computationally highly demanding evaluation of two-electron integrals as they occur in the original formulation [1].
We present a reformulation of the frequency-independent Breit interaction operator in spherical coordinates and derive the corresponding matrix elements over spinors [2]. With this formulation it becomes possible to compute the matrix elements of the Breit interaction efficiently and analogously to those of the Coulomb interaction, i.e., by determining the corresponding interaction potential functions using Poisson equations.
The derived formulae will equally simplify computations using either basis-sets or a numerical representation of the orbitals such that the Breit interaction can be included efficiently in CI and SCF calculations for atoms and molecules. Of course, the computation of the Breit contribution to the total electronic energy as a first-order perturbation correction is also simplified. Furthermore, the frequency-dependent Breit interaction can be treated analogously.

[1] I. P. Grant, N. C. Pyper, *J. Phys. B*, 9 (1976) 761, [2] M. Reiher, J. Hinze, *J. Phys. B*, submitted