Spin at the 2-component level of theory. The way in pain

L. Bučinský[1], M. Malček[1], S. Biskupič[1], J. Kožíšek[1], D. Jayatilaka[2], V. B. Arion[3], G. E. Büchel[3]

[1]Institute of Physical Chemistry and Chemical Physics FCHPT, Slovak University of Technology, Radlinskeho 9, Bratislava, SK-812 37,Slovakia

[2]Department of Chemistry, University of Western Australia, 35 Stirling Hwy, Crawley WA 6009, Australia

[3]University of Vienna, Institute of Inorganic Chemistry, Währinger Str. 42, A-1090 Vienna, Austria

lukas.bucinsky@stuba.sk

It will be shown that a non-relativistic unrestricted 2-component (2c) calculation of an open shell system can break the $\hat{S}_z$ "symmetry" as it is the case for a quasirelativistic unrestricted 2c calculation. Although spin itself cannot be regarded as a constant of motion at the 2c level of theory, especially when the spin-orbit coupling is accounted for, an analog of the spin contamination for an unrestricted 2c wave function will be presented. The 2c analog of the spin contamination will be evaluated by means of the overlap between the set of the original spinorbitals and the appropriate Kramers spinorbital set [1]. The comparison between the 1-component and 2-component spin density representations [2, 3, 4, 5, 6] will be presented. A "Kramers unrestricted" analog of spin density, which is based on the overlap between the original spinor set and the Kramers spinor set, will be introduced [1].

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