Relativistic correlation

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Fundamental breakthroughs have recently been achieved in relativistic quantum chemistry based on the no-pair Dirac-Coulomb-Breit Hamiltonian (for a recent review see Ref. [1]). However, there still exist two issues that require great attention, i.e., how to go beyond the no-pair approximation so as to account for the correlation contributions of negative energy states and how to do relativistic explicit correlation under the no-pair approximation. It turns out[2] that the QED prescription must be invoked for the former case while an extended no-pair projection has to be introduced for the latter case.

Bibliography:

1. W. Liu, Mol. Phys. **108**, 1679-1706 (**2010**).
2. W. Liu, Phys. Chem. Chem. Phys. (submitted).