Exact infinite–order two–component theory for relativistic quantum chemistry

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A method for the generation of the numerically exact two–component hamiltonian for the use in relativistic quantum chemistry is presented. With appropriately selected basis sets the method is shown to give the exact Dirac energies. The complete separation of the electronic and positronic states is accomplished by a simple iterative scheme. The proposed method shows that all of relativistic quantum chemistry can be done in the framework of the two–component formalism. If needed, the positronic states can be separately determined in a similar way. Thus, the present method can be also used for the evaluation of quantum electrodynamic corrections in the finite basis set approximation.