Quasidegenerate relativistic direct perturbation theory and effective Hamiltonians for electrons

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The construction of an effective Hamiltonian for quasidegenerate direct perturbation theory of relativistic effects is presented. It is based on a transformation of the Dirac Hamiltonian, that decouples both electronic from positronic states and states inside the model space from those outside of it. The formalism of Rutkowski and Schwarz is contained in the new theory as a special case. A generalization to infinite order, i.e. a non-perturbative iterative approach is also possible. The new formalism is particularly suited for relativistic perturbation theory applied to the MC-SCF method. Some preliminary results are presented.