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Towards the self-energy correction of the no-pair Dirac−Coulomb energy for two-electron systems

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Among the leading Quantum Electrodynamical (QED) corrections to atomic-molecular energy levels, the effect of one-loop electron self-energy has proven to be one of the most challenging to compute.
There are well-established techniques to calculate it in two extreme cases (for predominantly non-relativistic[1] and highly relativistic[2] systems, like low-charged and highly charged ions, respectively), but no general method to a correlated relativistic reference state is known.

Finding a self-energy calculating approach generally applicable regardless of the strength of relativistic effects is part of our ongoing research effort to build QED corrections on highly accurate relativistic two-particle wave functions[3]. Our starting point is the equal-time formulation of the Bethe−Salpeter equation[4], and its first approximation, the no-pair Dirac−Coulomb(−Breit) equation; radiative and non-radiative QED corrections are then included perturbatively.

In my poster, I present our current progress towards the calculation of self-energy with a relativistic two-electron wave function. The reference is a no-pair Dirac−Coulomb wave function obtained from an explicitly correlated variational procedure, providing an all-order description of (instantaneous, non-radiative) relativistic effects[5].
Working in the framework of the dipole approximation while using such a reference leads to a simple relativistic extension of the so-called Bethe logarithm, and endows the low-frequency part of the self-energy (plus transverse photon exchange) with higher-order binding corrections[3]. An example calculation is given for the ground state of the helium atom.
Moving beyond the dipole approximation raises several questions concerning the renormalization, the role of negative-energy states and permutational symmetry issues of inner states. A fully numerical renormalization scheme is proposed, reminiscent of partial wave renormalization[2]. The new challenges and obstacles associated with the relativistic treatment of self energy beyond the dipole approximation are discussed, with preliminary numerical results.

References

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