Geminals in Dirac-Coulomb Hamiltonian eigenvalue problem

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The Dirac-Coulomb (DC) Hamiltonian is a rather strange hybrid composed of a relativistic one-body part and a non-relativistic two-body interaction term. The evolution equation of a system described by this Hamiltonian is neither Galileo nor Lorentz invariant. The bound and the continuum states derived from the DC Hamiltonian eigenvalue equation are coupled by the electron-electron interaction and, from the formal point of view, the eigenstates corresponding to physically bound states (e.g. to the ground state of the helium atom) are resonances. As a consequence of these difficulties, some authors argue that one should abandon the DC equation as a target for variational approaches and treat it using perturbation-type methods only. On the other hand, the DC equation constitutes a starting point to the development of numerous variational approaches, which are commonly (and successfully) used in practical calculations. Therefore, the knowledge on the variational properties of this equation is essential and its accurate variational solutions form important benchmarks. However, the variational treatment of the DC equation has to be performed with a great care.

In this presentation several modes of application of the Hylleraas-CI method to solving the DC Hamiltonian eigenvalue problem are reported. The influence of the non-separability of the geminal part of the trial function on the form of the constrains imposed upon the variational space is discussed in detail. In particular, the relations between the approaches utilizing constrains derived from the so called kinetic balance condition and the ones based on the positive-energy-projected no-pair form of the DC Hamiltonian is discussed. It is also shown, that the coupling of the bound states to the continuum (usually referred to as the Brown-Ravenhall disease) may be efficiently treated using the complex coordinate rotation method. As an illustration of the approach, the results of calculations of the ground state energies of helium-like atoms are analysed.

References

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