Heavy atoms' calculations at the edge of accuracy: from high-precision spectroscopy to tests of fundamental physics.

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The progress on the development of novel methods for precision calculation of properties of heavy atomic systems with a few valence electrons is reported. The methods combine size-extensive all-order approaches used for the treatment of dynamic electron correlation with the "dressed" configuration interaction approach, which is particularly suitable for the efficient description of non-dynamic correlation effects in heavy many-electron systems, described by Dirac-Coulomb-Breit Hamiltonian. The novel methods can also incorporate the extrapolated intermediate Hamiltonian (XIH) techniques [1] and has several methodological and computational advantages, based on opportunity to make different extrapolation procedures proceeding from the approximate intermediate Hamiltonian to the precise effective Hamiltonian. Development of the methods are aimed at significant improvement in the theoretical accuracy of spectra and different non-energetic physical properties, including various nuclear and parity non-conservation effects, as well as variation of fundamental physical constants. Presented elaborated energy spectra calculations, tests of fundamental symmetries and other applications not only require precise high-level techniques, but also evaluation of the accuracy of the results. Excellent agreement with experiment (when available) and significant improvement compared with traditional single and multireference coupled cluster approaches is obtained (for recent reviews see [2-4]).

References:

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[3] E. Eliav and U. Kaldor, in "Recent progress in coupled cluster methods: Theory and Applications", eds. J. Pittner, P. Charsky and J. Paldus (Springer, 2010), p. 113.
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