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(UG*) Variational bound for the energy of the H-negative ion: Triple basis sets

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We report an improved variational upper bound for the ground state energy of H^- using Hylleraas-like wave functions in the form of a triple basis set having three distinct distance scales. The extended precision DQFUN of Bailey, allowing for 70 decimal digit arithmetic, is implemented to retain sufficient precision. Our result exceeds the previous record [1], indicating that the Hylleraas triple basis set exhibits comparable convergence to the widely used pseudorandom all-exponential basis sets, but the numerical stability against roundoff error is much better. It is argued that the three distance scales have a clear physical interpretation. The new variational bound for infinite nuclear mass is $-0.527\ 751\ 016\ 544\ 377\ 196\ 590\ 814\ 478$ a.u. [2]. New variational bounds are also presented for the finite mass cases of the hydrogen, deuterium and tritium negative ions H^- , D^- and T^- , including an interpolation formula for the mass polarization term.

[1] A. M. Frolov, Euro. J.Phys. D 69, 132 (2015).

[2] E. M. R. Petrimoulx, A. T. Bondy, E. A. Ene, Lamies A. Sati, and G. W. F. Drake, Can. J. Phys. in press (2024).

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Hydrogen negative ion H^-

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Keyword-3

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