Abstract Submitted
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High precision variational calculations of non-relativistic energy levels of the hydrogen molecular ion[1] YE NING, ZONGCHAO YAN, University of New Brunswick — We have performed a benchmark calculation of non-relativistic energy level of H_2^+, using Hylleraas coordinates [1] containing three non-linear parameters so that three inter-particle radial coordinates r_1, r_2, and r_{12} can be described independently. Rayleigh-Ritz variational principle is used to find out minimum of the expectation value of Hamiltonian of this system. Configuration of base varies according to the total angular momenta J of the system, the bigger J is, the more blocks are needed. To solve the matrix equation, power method is used to identify the ground state as well as some other excited states. The non-relativistic ground state energy of H_2^+ has been calculated to a few parts in 10^{33}, which represents the best energy level reported so far.

[1] M. M. Cassar and G. W. F. Drake, *J. Phys. B.* **37** 2485 (2004)

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