Relativistic corrections for the ground state of the hydrogen molecule

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The Schrödinger equation for the ground state of the hydrogen molecule is solved by the Rayleigh-Ritz variational method in Hylleraas coordinates without using the Born-Oppenheimer approximation. The non-relativistic energy eigenvalue converges to $-1.164\,025\,030\,4(5)$ a.u.. Then the leading order relativistic corrections (including the mass-velocity, Darwin, orbit-orbit, and spin-spin terms) and the relativistic recoil terms are calculated by perturbation method. Together with the QED corrections and higher-order corrections calculated by M. Puchalski, J. Komasa, and K. Pachucki [1], we obtain the dissociation energy of the hydrogen molecule $D_0 = 36\,118.069\,47(47)$ cm^{-1}, which agrees with the recent experimental results $36\,118.069\,62(37)$ cm^{-1} [2] and $36\,118.069\,45(31)$ cm^{-1} [3].

Table 1: The non-relativistic energy eigenvalue, the α^2 correction, and the α^2 contribution to the dissociation energy for the ground state of the hydrogen molecule.

Basis size	Non-relativistic energy (in a.u.)	α^2 correction (in 10^{-5} a.u.)	α^2 contribution to the dissociation energy (in cm^{-1})
256	–1.163 966 582 92	–1.088 999 4	–0.531 751
500	–1.164 014 701 97	–1.091 203 3	–0.526 914
912	–1.164 022 742 55	–1.090 704 3	–0.528 009
1570	–1.164 024 408 23	–1.090 057 1	–0.529 429
2570	–1.164 024 831 12	–1.089 629 1	–0.530 369
4050	–1.164 024 974 62	–1.089 440 2	–0.530 783
6150	–1.164 025 011 35	–1.089 361 0	–0.530 957
9070	–1.164 025 022 86	–1.089 315 7	–0.531 056
13020	–1.164 025 027 14	–1.089 288 1	–0.531 117
18270	–1.164 025 028 91		
25100	–1.164 025 029 71		
33870	–1.164 025 030 10		
Extrap.	–1.164 025 030 4(5)	–1.089 24(5)	–0.531 21(10)

[1] M. Puchalski, J. Komasa, and K. Pachucki, Phys. Rev. A **95**, 052506 (2017).
[2] J. Liu *et al.*, J. Chem. Phys. **130**, 174306 (2009).
[3] R. K. Altmann *et al.*, Phys. Rev. Lett. **120**, 043204 (2018).