

Abstract Submitted
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Long-range asymptotic behaviour of the exchange energy in the hydrogen molecule MICHAL SILKOWSKI, KRZYSZTOF PACHUCKI, University of Warsaw — The exchange energy is of fundamental importance for the understanding of interatomic interactions. Its long-range behavior in H_2 was investigated in the early days of quantum mechanics¹. Those results were met with criticism² and asymptotically correct form was derived by Herring and Flicker³. Despite further work by many authors^{4,5}, long-range asymptotics of exchange energy in H_2 still raises controversy.

We present high-precision variational calculations of energy splitting between the lowest hydrogen states performed with our H2SOLV⁶ package, which utilizes explicitly correlated exponential basis⁷. Due to correct asymptotic behavior of our basis, we claim that our numerical results resolve this controversy.

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Michal Silkowski
University of Warsaw

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