

The Hydrogen benchmark project: equation of state with state-of-the-art many-body methods

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I will describe the hydrogen benchmark project by the Simons Collaboration on the Many-Electron Problem. We obtain numerical results for the equation of state of an infinite chain of hydrogen atoms. A variety of modern many-body methods are employed, with exhaustive cross-checks and validation. Approaches for reaching the continuous space limit and the thermodynamic limit are investigated, proposed, and tested. The detailed comparisons provide a benchmark for assessing the current state of the art in many-body computation, and for the development of new methods. The ground-state energy per atom in the linear chain is accurately determined versus bondlength, with a confidence bound given on all uncertainties [1]. I will then briefly discuss on-going efforts to determine the phase diagram of the hydrogen chain.

[1]. Mario Motta, et. al., arXiv:1705.01608 (2017).