Hydrogen Equation of State at planetary conditions through Variational Quantum Monte Carlo

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ABSTRACT

Hydrogen is the lightest and most abundant element in the Universe and plays a pivotal role in gas giant planets such as Jupiter. Despite its elemental simplicity, hydrogen exhibits a complex phase diagram due to strong electron-electron correlations. Accurately modelling the interior of gas giant planets requires an equation of state (EOS) for hydrogen with an error on the order of 1% [1]. However, current experimental techniques fall short of achieving the necessary pressures, while state-of-the-art density functional theory (DFT) calculations are limited in accuracy due to assumptions regarding electron exchange-correlations. To address the challenge, we compute hydrogen EOS at different levels of theory to understand how much the choice of the assumptions affects the final result, and if this level of uncertainty is adequate for planetary science. To do so we employ several exchange-correlation functionals within DFT and Variational Quantum Monte Carlo (QMC), a theoretical modelling approach that can improve the description of electrons correlation, making it ideal for studying hydrogen at gas giant planets conditions. Notably, recent studies have demonstrated the remarkable agreement between QMC and hydrogen Hugoniot data [2]. To overcome the computational cost of QMC Molecular Dynamic (MD), we adopt a sampling strategy employing DFT MD simulations based on the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional. This strategy enables the extraction of uncorrelated configurations, allowing for more efficient calculation of internal energy and pressure using QMC, and then compute the EOS using re-weighting technique [3]. Our results exhibit excellent agreement with full QMC-MD simulations reported in [4]. We observe that, as expected, the choice of theory drastically impact the EOS: specifically, QMC predicts a denser EOS, suggesting the envelope of Jupiter to be poor in heavy element and pointing out the difficulty in understanding Jupiter's current structure and origin.

References

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