Development of a new highly-accurate equation of state for hydrogen and the hydrogen-helium mixture

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The equation of state (EOS) of the hydrogen-helium mixture is an important input in the astrophysical modeling of stars, in particular our Sun, and of giant planets. A highly-accurate EOS is needed in particular to fully exploit the data provided by heliosismology. The needed accuracy cannot be reached within the chemical approach, in which the gas is described as made up of particles of different chemical species like free electrons and protons, atoms H and He, ions He^+, H_2^+, ..., but requires the use of the physical approach. The studied gas is thus described as made up of its three basic constituents, namely electrons, protons and helium nuclei, which are all treated as quantum point particles interacting solely via the Coulomb interaction. The OPAL equation of state has been derived in this framework, but it uses some approximations and modelizations and it is available only in the form of precomputed numerical tables [1].
I will present a new equation of state [2] for a partially ionized hydrogen gas derived within the Ring Polymer Representation of the gas at finite temperature which follow from rewriting the system's partition function in terms of Feynman path integrals. This so-called “Scaled Low Temperature” (SLT) EOS takes the form of a systematic and approximation-free expansion around the ideal-gas Saha equation of state. It involves, as an important ingredient, few-body cluster functions that account for non-ideal effects associated to groups of close-by particles, in particular the formation and excitation of atomic and molecular bounds states. A cluster function depends solely on the temperature T and has the form of a truncated trace $\mathrm{Tr}(\exp(-H_{NpNe}/kT)\text{-}...)$ where H_{NpNe} is the Coulomb Hamiltonian for N_p protons and N_e electrons and where the subtracted terms in the ellipsis ensure the convergence of the trace. We have computed numerically those cluster functions, which are closely related to usual virial coefficients, by using a Path Integral Monte Carlo approach [3]. Efficient Monte Carlo sampling of those functions is achieved, even at quite low temperatures (kT<<Rydberg) where bound states can form, thanks to the introduction of an importance sampling function. We have introduced furthermore an adaptive scheme for the discretization of the particle paths which is more efficient than the traditional uniform discretization. Numerical results for the predictions of the SLT EOS, with comparisons to other approaches such as OPAL, will be presented.

[1] F. J. Rogers, F. J. Swenson, and C. A. Iglesias, *Astrophys. J.* **456**, 902 (1996).
[2] A. Alastuey and V. Ballenegger, *Phys. Rev. E* **86**: 066402 (2012)
[3] D. Wendland, V. Ballenegger, and A. Alastuey, *J. Chem. Phys.* **141**, 184109 (2014)