Equation of state for a hot hydrogen gas from path integral Monte Carlo calculations of cluster functions

Vincent Ballenegger
Institut UTINAM, Université de Bourgogne - Franche-Comté, 25030 Besançon

We study the thermodynamics of a partially ionized hydrogen gas within the physical picture where the system is described as a gas of quantum point electrons and protons interacting solely via the Coulomb potential. An exact expansion for the thermodynamic properties of the gas is derived in a scaling limit at low temperatures and low densities. The analysis is performed using the known mapping of a quantum system onto a classical system of interacting ring polymers. Our expansion involves cluster functions, which are analogous to usual (temperature-dependent) virial coefficients, that describe the contributions to the equation of state of small clusters of particles. The cluster functions account in particular for the formation of atomic and molecular bound states. We use a path integral Monte Carlo algorithm with importance sampling to compute those cluster functions accurately. Results for the cluster functions and for the thermodynamical properties of the hydrogen gas will be presented.