Nature of the Hydrogen Plasma Phase Transition

Kris Delaney\(^{(1)}\), David Ceperley\(^{(1)}\), Carlo Pierleoni\(^{(2)}\)

(1) Department of Physics, University of Illinois at Urbana-Champaign
(2) Dipartimento di Fisica, Università del L’Aquila, L’Aquila, Italy

We present details of a study of pure hydrogen fluid at high pressures. Using the Coupled Electron-Ion Monte Carlo (CEIMC) method [1,2], a quantum Monte Carlo scheme capable of accurately simulating systems at low temperature, we study the nature of the plasma phase transition; the mechanism by which a purely molecular fluid transforms into a non-molecular fluid under increasing pressure.

The CEIMC method centers on exploring the nuclear configuration space (classically or with quantum path integrals) using a modified Metropolis algorithm, with configurational energy differences computed from Born-Oppenheimer energies. Energy differences are computed with VMC or Reptation quantum Monte Carlo, both of which supply unbiased estimates of energy differences, the latter within a projector framework.
