

Abstract Submitted
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The Nature of the Hydrogen Plasma Phase Transition KRIS DELANEY, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, Università del L'Aquila, Italy — We present details of a study of pure hydrogen fluid at high pressure. 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 (PPT): the mechanism by which a molecular to non-molecular transformation occurs under increasing pressure. We find no evidence for a first-order PPT. The CEIMC method centers on exploring the nuclear configuration space (classically or with quantum path integrals) using a modified Metropolis algorithm. Configurational energy differences are computed within the Born-Oppenheimer (BO) approximation using accurate ground-state quantum Monte Carlo techniques.

1. D. Ceperley, M. Dewing and C. Pierleoni, in *Bridging Time Scales: Molecular Simulations for the Next Decade*, eds. P. Nielaba *et al*, Springer-Verlag, pgs. 473-500 (2002).
2. C. Pierleoni, D. M. Ceperley and M. Holzmann, *Phys. Rev. Lett.* **93**, 146402 (2004)

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