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Coupled Electron-Ion Monte Carlo Study of Hydrogen KRIS DELANEY, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, Dipartimento di Fisica, Università del L'Aquila, L'Aquila, Italy — We present details of the Coupled Electron-Ion Monte Carlo method (CEIMC) [1,2] applied to the problem of the equation of state of pure hydrogen. The aim is to develop a method that can predict state information outside the range of temperatures and pressures that are accessible with other existing methods, such as PIMC.
The CEIMC method centers on exploring the configuration space of the hydrogen nuclei (classical or 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. New developments include a fast band-structure calculation for the trial function which should improve the localization of molecule-atom phase transitions.
(1) D. Ceperley, M. Dewing and C. Pierleoni, in Bridging Time Scales: Molecular Simulations for the Next Decade, eds. P. Nielaba, M. Mareschal and G. Ciccotti, 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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