"Path Integral Simulation of Hot, High Pressure Hydrogen"

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ABSTRACT

Fermionic path integral Monte Carlo simulations have been applied to study the equilibrium properties of the hydrogen in the Mega-bar regime corresponding to the density and temperature range of $0.001 < P < 0.5$ g/cc and $5000K < T < 1000000K$. We determine the equation of state and the phase diagram, study ionization and dissociation effects and discuss the regime where a plasma phase transition has been predicted in hydrogen. We compare two different nodal surfaces taken from the free particles and from a variational density matrix (1) and estimate the effect on the thermodynamic variables. Furthermore we calculate the Hugoniot function and compare with Laser shock wave experiments (2). Finally, simulations with open paths will be described that can be used to determine the momentum distribution of the electron gas at finite temperature.

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More details at: http://www.ncsa.uiuc.edu/Apps/CMP/militzer/research.html

(1) B. Militzer, E. L. Pollock, "Variational Density Matrix Method for Warm Condensed Matter and Application to Dense Hydrogen", in press, Phys. Rev. E (2000).

(2) B. Militzer, D. M. Ceperley, "Path Integral Monte Carlo Calculation of the Deuterium Hugoniot", submitted to Phys. Rev. Lett. (2000).