Quantum Monte Carlo Simulations of Dense Hydrogen

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Abstract:

Quantum Monte Carlo (QMC) methods are among the most accurate, general methods for computing total electronic energies. However, they have been limited to temperatures greater than 5000K, or to zero temperature. In recent years, we have been developed a method Coupled Electron-Ion Monte Carlo, to allow coupled simulations of correlated electrons and ions. We use both trial wave functions that depend analytically on the ionic coordinates, as well as those from a band structure calculation. Reptation MC is used for accurate calculation of the BO energy differences[1]. The quantum effects of the ionic degrees of freedom and the boundary conditions on the phase of the wavefunction can be integrated over with a modest increase in computational effort.

We have performed simulations of dense hydrogen down to temperatures of 300K. Our results show features of the phase diagram qualitatively different than computed using DFT, for example, in the melting of the atomic solid[2] and in the atomic-molecular transition in the dense liquid[3]. The equation of state of dense hydrogen differs significantly from that of Saumon and Chabrier in the region of the atomic-molecular transition.

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3. K. Delaney, C. Pierleoni and D. M. Ceperley, cond-mat/0603750.