Quantum Monte Carlo Simulations of Dense Hydrogen

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Abstract

Quantum Monte Carlo (QMC) methods are the most accurate and general methods for computing total electronic energies. However, in general, they have been limited to high temperatures or to zero temperature. In recent years, we and others have been working on methods that utilize the Born Oppenheimer approximation to allow simulations coupling the correlated quantum systems and a system of ions. Using quantum Monte Carlo, one estimates the Born-Oppenheimer energy change for a movement of the ions which is then used in a Monte Carlo simulation of the ionic degrees of freedom. The quantum effects of the ionic degrees of freedom and the boundary conditions on the phase of the wavefunction can be integrated over. 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 and in the atomic-molecular transition in the liquid.