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Quantum Monte Carlo Simulations of Warm Dense Hydrogen[1]

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Quantum Monte Carlo 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 [1] 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. We have used this method to determine the equation of state of warm dense hydrogen, to study the cross-over from the molecular liquid to the atomic liquid [2] and for the melting temperature of solid atomic hydrogen [3].

[1] C. Pierleoni and D. M. Ceperley, ChemPhysChem 6, 1 (2005); physics/0501013.
[2] K. Delaney, C. Pierleoni and D. M. Ceperley, Phys. Rev. Letts. 97, 235702 (2006).
[3] C. Pierleoni, D. M. Ceperley and M. Holzmann, Phys Rev. Letts. 93, 146402 (2004).

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