Abstract Submitted
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Path Integral Quantum Monte Carlo Benchmarks for Molecules and Plasmas[1] JOHN SHUMWAY, Arizona State University — Path integral quantum Monte Carlo is used to simulate hot dense plasmas and other systems where quantum and thermal fluctuations are important. The fixed node approximation—ubiquitous in ab initio ground state Quantum Monte Carlo—is more complicated at finite temperatures, with many unanswered questions. In this talk I discuss the current state of fermionic path integral quantum Monte Carlo, with an emphasis on molecular systems where good benchmark data exists. We look at two ways of formulating the fixed node constraint and strategies for constructing finite-temperature nodal surfaces. We compare different the free energies of different nodal choices by sampling an ensemble of nodal models within a Monte Carlo simulation. We also present data on imaginary-time correlation fluctuations, which can be surprisingly accurate for molecular vibrations and polarizabilty.

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