

# *Ab Initio* Finite Temperature Auxiliary Field Quantum Monte Carlo

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Predicting finite temperature (FT) properties of molecules and solids is critical to understanding many physical and chemical processes. However, developing accurate, yet efficient theoretical approaches for FT applications remains an outstanding challenge. Aside from FT mean field theories that have limited accuracy and FT Full Configuration Interaction with exponential scaling, proper ways to generalize various ground state post Hartree-Fock theories to FT is still an open problem. Furthermore, FT generalizations of density functional theory, considered to be promising candidates for future large scale simulation, require additional benchmarking against more accurate methods. We present an auxiliary field quantum Monte Carlo method for studying the electronic structure of molecules and solids at finite temperature. Excellent agreement within chemical accuracy is achieved compared to exact diagonalization across a wide range of temperatures for various model and *ab initio* systems. The fermion sign problem (or, more generally, the phase problem) is effectively controlled, even at very low temperature, through importance sampling and the phaseless approximation. Our method provides an additional tool to study low temperature physics and ultracold chemistry.