Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo for Solids

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Predicting the finite temperature properties of molecules, and especially, solids is critical for understanding many chemical and physical phenomena. Nevertheless, developing accurate, yet efficient methodologies for finite temperature applications remains an outstanding challenge. In this work, we present an Auxiliary Field Quantum Monte Carlo method with an $O(N^3)$ scaling for studying the finite temperature electronic structure of any system that can described by an *ab initio* Hamiltonian.[1] The algorithm marries the *ab initio* phaseless auxiliary field quantum Monte Carlo algorithm known to produce high accuracy ground state energies of molecules and solids with its finite temperature variant, long used by condensed matter physicists for studying model Hamiltonian phase diagrams, to yield a phaseless, *ab initio* finite temperature method. We demonstrate the accuracy of this approach for benchmark molecules, including the carbon dimer, and solids, including hydrogen chains and networks, and compare it to more popular mean field treatments of real materials. Our method serves as a new, robust tool for studying low, but finite temperature phase transitions in models and solids, ultracold chemistry, and warm dense matter.

References

1. Y. Liu, M. Cho, and B. M. Rubenstein. *JCTC*. **14** (2018), 4722.