Finite Temperature Density Matrix Embedding Theory[1] CHONG
SUN, GARNET CHAN, Caltech — *Density Matrix Embedding Theory* (DMET) provides a powerful and less expensive framework to treat strongly correlated ground-state problems in both solids and molecules, by reproducing the entanglement between the fragment and its environment at mean-field level, while the fragment is treated at a more accurate level. In this talk, I will extend the ground-state DMET to finite temperature DMET (FT-DMET), by solving both the mean-field problem and impurity problem at finite temperature T, and reconstructing bath orbitals from the mean-field solution. The finite temperature Lanczos algorithm as an alternative of full configuration interaction (FCI) is used to implement the impurity solver, and a cutoff is introduced to the selection of bath orbitals from the mixed mean-field solution. We assess the performance of FT-DMET by several benchmark calculations on both molecules and lattices. The results are compared to other well-established finite temperature methods, such as quantum Monte Carlo (QMC), dynamical mean-field theory (DMFT), and so forth.

[1]Simons Foundation

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