

A novel impurity solver in dynamical mean field theory:

Iterative perturbation theory combined with the parquet equations

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Although several impurity solvers in dynamical mean field theory (DMFT) [1] have been proposed, there are practical difficulties arising from a trade-off between numerical costs and reliability, especially in multi-band systems. In this study, we re-interpret the iterative perturbation theory (IPT) [2] as an approximation that captures the strong correlation effects by mimicking the particular frequency structures of the exact two-particle vertex. From this insight, we extend IPT, by combining it with the parquet equations, such that it has efficiency and reliability simultaneously. We apply this method to several models to evaluate the validity. We confirm that our method shows good agreement with the numerically exact continuous-time quantum Monte Carlo method (CT-QMC)[3], not only in single-band systems, but also in multi-band systems. In this presentation, we will explain the details of the method and show the results of benchmarks.

References

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