Methodological improvements for hybridization expansion continuous-time quantum Monte Carlo simulations - Polynomial basis representation of observables and improved estimators -

Dr. Hartmut Hafermann
(Centre de Physique Théorique, École Polytechnique
CNRS, F-91128 Palaiseau Cedex, France)

Abstract:

The hybridization expansion continuous-time quantum Monte Carlo algorithm is an efficient and flexible tool for the solution of multiorbital Anderson impurity models. In this talk, I will address two recent methodological improvements for this algorithm: The first is a representation of imaginary-time Matsubara Green functions in terms of Legendre orthogonal polynomials. Single- and two-particle Green functions can be directly measured in this basis, which results in a compact representation of these objects. In addition, this representation acts as an efficient noise filter.

The second addresses the problem of large errors in the intermediate and high-frequency behavior of the self-energy when computed from Dyson's equation. A similar problem occurs for the vertex function. It is shown that these problems are solved using improved estimators which are based on higher-order impurity correlation functions. In the segment representation, the improved estimators can be accumulated at essentially no additional computational cost. Combined with the Legendre noise filter, the method yields very accurate estimates for the self-energy and vertex function over the full frequency range and improves the stability of analytical continuation procedures.

References:

Lewin Boehnke, Hartmut Hafermann, Michel Ferrero, Frank Lechermann, and Olivier Parcollet, Orthogonal polynomial representation of imaginary-time Green’s functions, Phys. Rev. B 84, 075145 (2011).

Hartmut Hafermann, Kelly R. Patton and Philipp Werner, Improved Estimators for the Self-Energy and Vertex Function in Hybridization Expansion Continuous-Time Quantum Monte Carlo Simulations, arXiv:1108.1936 (Phys. Rev. B, in print).