

Two-particle self-consistency in diagrammatic theories for strongly correlated electron systems

Short abstract

Materials with partially filled d - or f -shells often exhibit fascinating physical properties such as magnetism or high-temperature superconductivity. Many of these phenomena originate from strong electron correlations, making their theoretical description highly challenging. Over the last 30 years, significant progress has been achieved through dynamical mean field theory (DMFT), which captures all local correlations. This approach has provided the first quantitative understanding of the correlation-driven Mott-Hubbard metal-to-insulator transition in transition metal oxides [1]. However, much of the remarkable physics of correlated electrons on a lattice stems from—or is at least strongly influenced by—non-local correlation effects. To include these in the theoretical framework, several so-called “diagrammatic extensions” of DMFT have been developed over the last decade [2]. Although these approaches have captured non-local effects such as the pseudogap phase in high-temperature superconducting cuprates [3], several open questions remain: (i) The predictive power of virtually all diagrammatic extensions of DMFT is limited by intrinsic inconsistencies in the calculation of physical observables, such as kinetic and potential energies. (ii) These theories are currently restricted to simple single-band model systems, such as the Hubbard Hamiltonian, and (iii) the origin of differences in results produced by different flavors of these diagrammatic extensions remains unexplained. These issues are being addressed by the Emmy Noether project, “Two-particle self-consistency in diagrammatic theories for strongly correlated electron systems” (<https://gepris.dfg.de/gepris/projekt/407372336>) of the Deutsche Forschungsgemeinschaft (DFG). The project requires extensive numerical simulations, which are only feasible within manageable time scales using sufficiently large high-performance computing systems such as the NHR.