Ab initio Dynamical Vertex Approximation

Project	Ab initio Dynamical Vertex Approximation
Project acronym	ABINITIODGA
Researcher (PI)	Karsten Held
Host institution (HI)	TECHNISCHE UNIVERSITAET WIEN, ÖSTERREICH
Call details	ERC-2012-StG, PE3
Summary	Some of the most fascinating physical phenomena are experimentally observed in strongly correlated electron systems and, on the theoretical side, only poorly understood hitherto. The aim of the ERC project AbinitioDGA is the development, implementation and application of a new, 21th century method for the ab initio calculation of materials with such strong electronic correlations. AbinitioDGA includes strong electronic correlations on all time and length scales and hence is a big step beyond the state-of-the-art methods, such as the local density approximation, dynamical mean field theory, and the GW approach (Green function G times screened interaction W). It has the potential for an extraordinary high impact not only in the field of computational materials science but also for a better understanding of quantum critical heavy fermion systems, high-temperature superconductors, and transport through nano- and heterostructures. These four physical problems and related materials will be studied within the ERC project, besides the methodological development. On the technical side, AbinitioDGA realizes Hedin's idea to include vertex corrections beyond the GW approximation. All vertex corrections which can be traced back to a fully irreducible local vertex and the bare non-local Coulomb interaction are included. This way, AbinitioDGA does not only contain the GW physics of screened exchange and the strong local correlations of dynamical mean field theory but also non-local correlations beyond on all length scales. Through the latter, AbinitioDGA can prospectively describe phenomena such as quantum criticality, spin-fluctuation mediated superconductivity, and weak localization corrections to the conductivity. Nonetheless, the computational effort is still manageable even for realistic materials calculations, making the considerable effort to implement AbinitioDGA worthwhile.
Website (HI)	http://www.tuwien.ac.at
Max ERC funding	1.49 million Euros
Duration	60 months