GW and DMFT

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Condensed matter physics can be formulated in terms of Green's functions describing the propagation of particles from one spacetime point to another. These propagators are determined by Hedin's equations and provide an alternative route to the electronic structure problem as conventionally employed mean-field theories (such as Hartree-Fock and density functional theory) using diagrammatic perturbation theory. This diagrammatic approach allows for estimates of the groundstate energy as well as the spectral properties of a system. Whereas for the former often the random phase approximation (RPA) within the adiabatic connection fluctuation-dissipation framework is applied, for frequency dependent observables two different approximations are usually used.

On the one hand, the GW approximation of the self-energy allows for accurate estimates of band gaps for weakly correlated systems and is strongly related to the RPA, because both approximations take only a specific topological class of diagrams (bubbles) into account. On the other hand, dynamical mean-field theory (DMFT) provides access to all topologically distinct, but local self-energy diagrams and is often used for strongly correlated systems. However, to describe realistic systems both, GW and DMFT should be combined. In this talk the merging of GW with DMFT is discussed with focus on the GW/RPA side and the ab initio computation of effective interaction parameters for the DMFT Hamiltonian. This includes low scaling algorithms for the GW and RPA as well as a constrained RPA scheme to determine the effective interactions in the strongly correlated subspace.