3.2 Characterization of Phase Transitions within the DMFT

In this section, we will discuss how phase transitions can be found and characterized within the DMFT. In subsection 3.2.1, we focus on the general implications of the mean-field character of the DMFT in connection with first-order transitions. A particularly important aspect is the question how the numerical stability of solutions in the iterative process is related to their thermodynamic (meta-) stability. This problem had been neglected in the literature so far and is now solved for a particular iteration scheme in subsection 3.2.2. Finally, we collect useful observables and discuss their general behavior in subsection 3.2.3.

3.2.1 Transitions of First or Higher Order

In a thermal statistical ensemble, properties such as the (free) energy per particle, average filling, or average double occupancy are defined in terms of traces over all possible states. Therefore, the observables are well-defined functions of a complete set of external parameters; for the Hubbard model on a given lattice (with unit variance of the DOS) these parameters are the on-site interaction U, the temperature T, and the chemical potential μ. More precisely, the free energy F is a continuous function while its derivatives may be discontinuous at some hypersurfaces, i.e., lines in a 2-dimensional subspace of parameters such as U and T. The discontinuities indicate a phase transition; according to Ehrenfest, the order of the transition is defined as the order of the first discontinuous derivative of F. In principle, the search for a phase transition is, therefore, straightforward: sweeping through the parameter space, one searches for jumps or kinks in the derivatives of F with respect to U or T, i.e., the double occupancy D or (minus) the entropy S or related observables. This is the usual practice, e.g., for QMC in finite dimensions.[6]

In contrast, in mean-field theories such as the DMFT, the ensemble average is performed with the mean-field [here $\mathcal{G}(i\omega_n)$, cf. subsection 1.2.3] as an additional parameter which has to be determined self-consistently. The resulting fixed point problem may have one or more solutions for each point in the original parameter space. In regions of the phase space where only one solution is known to exist or where the derivatives of F are found to be continuous, phase transitions can be pinpointed just like in direct methods by testing for higher order derivative discontinuities. If several solutions exist, however, the result of an iterative solution of the fixed point equations will depend on the initialization. For sequential solutions on a grid of phase points where the solution at one point initializes the iteration at the neighboring point, the solution within the coexistence region then depends on the sweeping direction: hysteresis occurs. For conserving approximations such as the DMFT, the free energy can be generalized as a Ginzburg-Landau functional F_{GL} of the physical parameters plus the mean field which agrees with the true free energy

[6] A serious complication for such methods based on the solution of finite size clusters is, however, the rounding of all phase transitions.