Classical and quantum phase transitions in strongly correlated electron systems

Dipl.-Ing. Thomas Schäfer

examiners: Prof. Dr. Karsten Held (TU Wien),
Prof. Dr. Walter Metzner (MPI Stuttgart)

August 10, 2016

Abstract

Strongly correlated electron systems exhibit some of the most fascinating phenomena of condensed matter physics. Beyond the famous example of the Mott-Hubbard metal-to-insulator transition and the occurrence of classical phase transitions like magnetic and charge ordering as well as superconductivity, quantum phase transitions in strongly correlated systems are currently under intense research. These transitions are quite intriguing, because they occur at zero temperature, where quantum fluctuations dominate the physics in contrast to their classical, thermal counterparts, but they affect broad sectors of the phase diagram of both real materials and model systems. Their theoretical description, however, faces big challenges, both analyt- ical and numerical, so that a comprehensive theory could not be established hitherto.

This dissertation aims at a theoretical understanding of classical and quantum phase transitions by exploiting cutting-edge field theoretical many-body methods: the dynamical mean field theory (DMFT), which treats local correlations, but neglects spatial correlations and the dynamical vertex approximation (DΓA), a diagrammatic extension of DMFT, which additionally incorporates spatial correlations on every length scale. These state-of-the-art methods are applied to one of the most important and fundamental model systems in condensed matter physics, the Hubbard model. First, precursor features of phase transitions are analyzed. They can, in fact, be of very different kind: In the case of the Mott-Hubbard transition they appear as divergent irreducible vertices, in the case of second order phase transitions as (charge-, spin- and pairing-) fluctuations. Then, the influence of the vicinity of second order phase transitions on one-particle spectra is investigated for various dimensionality. Interesting features of self-energies in specific dimensions are highlighted. In the next step, the fate of the Mott-Hubbard metal-insulator transition is determined for two dimensions, where the DMFT is known to become an inadequate approximation because it neglects spatial correlations. Eventually, the magnetic phase diagram of the doped Hubbard model in three dimensions (especially the region around its magnetic quantum critical point) is analyzed. The simultaneous treatment of strong local and non-local fluctuations makes DΓA particularly well suited to study the competing processes which control the physics of a strong-coupling quantum critical point. The DΓA critical exponents of the magnetic susceptibility and correlation length for the Hubbard model are determined, providing evidence for a significant violation of the prediction of the conventional Hertz-Millis-Moriya theory.

Length of abstract: $\sim$ 420 words
Length of dissertation: 192 pages