Mott-Hubbard Metal-Insulator Transition and Optical Conductivity in High Dimensions by Nils Blümer (Shaker Verlag, ISBN 3-8322-2320-7)

The characterization of a material as metallic or insulating, the study of transitions between such states, and the development of models for such transitions is of great fundamental and practical interest. The one-band Hubbard model is potentially relevant in this context since its primary parameter, the on-site interaction, triggers a transition or a crossover from metallic to insulating behavior at half filling. A reduction of complexity is achieved by the dynamical mean-field theory (DMFT); due to its nonperturbative character, this method is reliable in the range of interest, i.e., for intermediate to strong coupling. It becomes exact in the limit of high dimensionality (or large coordination number).

This work focuses on strongly correlated electron systems near a Mott metal-insulator transition. In the pedagogical chapter 1, we introduce the general electronic Hamiltonian and its reduction to the Hubbard model. We characterize the DMFT and its relation with mean-field approximations to spin systems and present the mean-field equations as well as their numerical solution using the auxiliary-field quantum Monte Carlo (QMC) method. Finally, we discuss the analytic continuation of imaginary-time Green functions by the maximum entropy method (MEM).

In chapter 2, we study the relations between lattice types, frustration, and densities of states (DOS). On the basis of Monte Carlo computations of momentum sums, we also evaluate the convergence of the DOS to its infinite-dimensional ($d = \infty$) limit. We present new insights on the "Bethe lattice" and on the impact of longer-range hopping for this model. A new formalism is developed that allows to construct models with hypercubic symmetry which reproduce an arbitrary target DOS in $d = \infty$. Using this approach, we can for the first time define a regular lattice with semi-elliptic DOS in $d = \infty$.

In the central chapter 3, we thoroughly explore the low-temperature properties of the fully frustrated Hubbard model with semi-elliptic DOS within the DMFT. The boundaries of a coexistence region of metallic and insulating solutions are determined with high accuracy, thereby resolving a controversy on the existence of a first-order transition within this model. We correct deficiencies in previously used QMC schemes and formulate an improved criterion for the detection of phase transitions. Going beyond previous work, the first-order transition line is accurately determined using a newly developed formalism. Finally, we suggest further methodological improvements and compute local MEM spectra with high precision.

Transport properties are discussed in chapter 4, where we review and extend the relevant formalisms. We derive new expressions for the optical f-sum rule in $d = \infty$. Fully lattice specific calculations of the optical conductivity are shown to be essential; errors made in earlier studies of frustration are quantified. We point out the ambiguities associated with any DMFT calculation of transport properties for "the Bethe lattice" and review possible concepts for making the problem well-defined; the regular lattice defined in chapter 2 is seen to have the most desirable properties. We then present accurate numerical results for the optical conductivity which are based on the MEM spectra computed in chapter 3.

The thesis closes with chapter 5, where we review the density functional theory and its local density approximation (LDA) and introduce the recently developed hybrid LDA+DMFT scheme. We discuss the solution using QMC as well as the extraction of photoemission and X-ray absorption spectra. Numerical results for the doped transition metal oxide $La_{1-x}Sr_xTiO_3$ with controlled precision are compared with experiments. Finally, a definition of the optical conductivity compatible with the LDA DOS is derived using the formalism developed in chapter 2; corresponding numerical results on the basis of MEM spectra are presented.