Chapter 1

Models and Methods

In this chapter we set the framework for the main part of this thesis by introducing the models under investigation and the approximations and methods employed. Studies of abstract models represent an idealized and focused view on physics which should be complemented by a clear knowledge about the inherent limitations. Therefore, we will emphasize those steps of abstraction from a “complete model” to the models studied in this work which potentially cause properties of the resulting theory to differ qualitatively from seemingly corresponding properties of real materials. Later, we will make contact with these observations, e.g., in the discussion of the f-sum rule of the optical conductivity (see chapter 4) and discuss a more complete picture in the context of the LDA+DMFT method and its application to $La_{1\text{-}x}Sr_xTiO_3$ in chapter 5. Since the density functional theory (DFT) and its local density approximation (LDA) are not central to this work, these approaches are introduced directly in the context of their application in chapter 5. As far as practical, methods like the quantum Monte Carlo (QMC) algorithm or the maximum entropy method (MEM) are covered here on a descriptive level while original methodological contributions are mainly discussed in the following chapters.

In the following, we will first discuss the Hubbard model in a general context in Sec. 1.1, then its nonperturbative treatment within the dynamical mean-field theory (DMFT) in Sec. 1.2. We describe the quantum Monte Carlo method of solving the DMFT self-consistency equations in Sec. 1.3 and the maximum entropy method of obtaining real-time dynamical information by analytic continuation of QMC imaginary-time data in Sec. 1.4.

1.1 Hubbard Model

The one-band Hubbard model is *the* minimal lattice model for strongly correlated electron systems, i.e., for describing electronic properties of materials which cannot be treated without explicitly taking the Coulomb interaction between the (valence) electrons into account. Typical examples are the transition metals and their compounds. In subsections 1.1.1 – 1.1.4, we explore the microscopic foundation of the Hubbard model and review some of its basic properties and limitations. Extensions of the one-band Hubbard model which can potentially overcome some of these limi-