Chapter 3

Mott Metal-Insulator Transition in the $d \to \infty$ Hubbard Model

One of the most fascinating phenomena of strongly correlated electron systems is the interaction-induced metal-insulator transition. Such a transition is fundamentally different from filling-induced transitions between metals and band insulators since it cannot be understood in terms of (effectively) noninteracting electrons. Particularly challenging is the Mott transition, the interaction-induced transition between a paramagnetic metal (PM) and a paramagnetic insulator (PI).[1] As this transition does not break the translational symmetry of the lattice, its description needs to take strong electronic correlations into account. For this reason, proximity to a Mott transition may be even regarded as a defining property of strongly correlated electron systems. The explanation and modeling of the Mott transition is a long-standing important and difficult problem of condensed matter physics (Mott, 1968; Mott, 1990; Gebhard, 1997; Imada, Fujimori, and Tokura, 1998).

In this chapter, we present studies of the Mott metal-insulator transition (MIT) occurring in the infinite-dimensional half-filled Hubbard model. Specifically, results will be obtained for the Bethe lattice, i.e., for a semi-elliptic noninteracting DOS. In order to observe the transition of interest in the paramagnetic phase, antiferromagnetism is suppressed in the calculation, which corresponds to treating the lattice as fully frustrated. For this model, the Mott transition occurs for an interaction U slightly larger than the bandwidth W (see below). Consequently, perturbative methods are not adequate for its description and may only a posteriori be useful for comparison. We will argue later that even numerically exact methods such as QMC or ED may become problematic in the transition region if not used with great care. In fact, one of the achievements of this thesis is the settlement of a controversy about the qualitative shape of the MIT phase diagram of the specified model. Therefore, our treatment will have to at least partially follow the historical development.

In Sec. 3.1 we give an experimental motivation and discuss the applicability of the model. In Sec. 3.2, we discuss strategies for pinpointing and characterizing phase

[1] Interactions can alternatively drive the transition of a metal into an insulating ordered state, namely an antiferromagnetic Néel low-temperature phase (AFI); the AFI, however, may be understood as an effective band insulator in the halved Brillouin zone (see subsection 1.1.4).