# Chapter 2

# Lattice and Density of States

Within the DMFT, properties of the lattice enter the computation of single-particle properties via the "noninteracting" density of states (DOS) $\rho(\epsilon)$ only.[1] Thus, in addition to the Hubbard interaction $U$, the temperature $T$, and the density $n$, the DOS constitutes an infinite set of input parameters for the DMFT treatment of the Hubbard model. While some aspects of a given DOS are easily characterized (with, e.g., the variance setting the energy scale for $U$ and $T$), many of its degrees of freedom may influence physical properties of the interacting system in a complicated way. More generally, the choice of hopping matrix elements or, equivalently, the choice of a dispersion $\epsilon_{\boldsymbol{k}}$ may be crucial for properties of Hubbard type models in any dimension. In most studies of the Hubbard model in dimensions $d > 1$, the hopping range has been restricted to nearest neighbors (NN) and, in some cases, next-nearest neighbors (NNN). While using only these largest hopping matrix elements is certainly a reasonable starting point, the remaining part can still be qualitatively important, in particular in high dimensions.

Three related problems motivate the studies presented in this chapter. First, up to now there has been no fully satisfactory way of treating the Hubbard model rigorously in $d = \infty$. As shown in Sec. 1.2, NN hopping on the hypercubic (hc) lattice leads to a Gaussian DOS without band edges in $d \to \infty$, which is unphysical since in the low-density limit the energy per electron becomes infinite and because an unbounded band violates the single-band assumption of energetically well-separated bands. Inclusion of NNN hopping not only leads to magnetic frustration and an asymmetric DOS but (for an appropriate sign of the hopping amplitudes) cures the problem of infinite energy in the low-density limit by introducing a sharp lower band edge in $d \to \infty$.[2] Another conventional way of establishing band edges in $d = \infty$ is taking this limit on the Bethe lattice which yields the semi-elliptic DOS used throughout chapter 3. Here, problems arise from the fact that the Bethe lattice is not a regular lattice but a treelike structure which has no loops and no well-defined

[1] The quotation marks, which we will drop from now on, are a reminder that (at least) interactions with lattice ions and core electrons are already included in the "noninteracting" dispersion $\epsilon_{\boldsymbol{k}}$ and, consequently, determine the "noninteracting" DOS.

[2] This cure is, however, not stable upon further extension of the hopping range: hopping to third-nearest neighbors generically reintroduces the low-energy tail extending to $\epsilon = -\infty$.