not restricted to small or large values of U. Since the theory is formulated in the thermodynamic limit, it yields continuous spectra and is per se free from finite-size problems. The local dynamics of the correlation problem, i.e., on-site correlations, are retained; only off-site short-range correlations are neglected. The mapping to a SIAM implies a considerable reduction in technical complexity. Still, the resulting problem is too complicated for a general analytic or computationally inexpensive numerical solution.

For a description of the MIT in $d = 3$ (where $1/Z$ has a value, e.g., of 1/6, 1/8, and 1/12 for the simple cubic, body centered cubic, and face centered cubic lattice, respectively) the limit of large coordination number seems a reasonable starting point. Only a nonperturbative method which keeps the local dynamical correlations can reliably characterize the MIT, since this transition is intrinsically an intermediate-coupling phenomenon (in contrast, e.g., to the transition to antiferromagnetic order which can be understood both at weak and strong coupling within perturbation theory). The thermodynamic limit is particularly important in the context of MITs as finite systems are always insulators. Provided that short-range fluctuations do not completely change the physics, we can hope to capture the essential correlation physics within the DMFT, at least when the impurity part is solved numerically exactly as in the QMC algorithm used throughout this work (see Sec. 1.3).

1.2.1 Limit $Z \to \infty$ for Spin Models

It has been known for a long time that the results of the Weiss mean-field approximation (Weiss, 1907) become exact for models with localized spins in the limit of infinite coordination number $Z \to \infty$ (Brout, 1960).[10] The Hamilton operator of the isotropic spin-1/2 nearest-neighbor Heisenberg model reads

$$\hat{H}_{\text{Heisenberg}} = -J \sum_{\langle ij \rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j = -J \sum_{\langle ij \rangle} \left(\hat{S}_i^z \hat{S}_j^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) \right) , \tag{1.15}$$

where the components of the spin operators obey the commutation rules $[\hat{S}_i^z, \hat{S}_j^\pm]_- = \pm\delta_{ij}\hat{S}_i^\pm$ and $[\hat{S}_i^+, \hat{S}_j^-]_- = 2\delta_{ij}\hat{S}_i^z$. In order for the energy per lattice site to remain finite when $Z \to \infty$, one has to scale the exchange interaction as $J = J^*/Z$, where J^* is independent of Z. Defining the average spin $\hat{\boldsymbol{h}}_i$ of the nearest neighbors (NN) of lattice site i,

$$\hat{\boldsymbol{h}}_i = \frac{1}{Z} \sum_{j \text{ NN of } i} \hat{\boldsymbol{S}}_j \, , \tag{1.16}$$

one finds that[11] $[\hat{\boldsymbol{h}}_i, \hat{\boldsymbol{h}}_j] = \mathcal{O}(1/Z)$(since only Z terms are nonvanishing) and that $\hat{\boldsymbol{h}}_i$ commutes with the Hamiltonian (1.15) to leading order (see, e.g., Gebhard, 1997).

[10]Note that Brout does not explicitly make the connection from the limit of infinite coordination number to the limit of infinite dimensionality but rather to the limit of infinite range of the exchange interaction which he assumes to be approached in the physical high-density limit of spin systems.

[11]Here and in the following, $\mathcal{O}(x^n)$ means "of the order of x^n", i.e., that the functional dependence on x (in the limit $x \to 0$) does not contain terms with lower powers than n.