The direct evaluation of the compressibility (as of most other susceptibilities) is numerically costly since it requires the QMC computation of 2-particle vertex functions. The formalism is omitted here since we will not show corresponding results; it can be found, e.g., in (Georges et al., 1996; Blümer, 1996). Spectra and optical conductivity data also shed light on systems near an MIT. Since due to numerical uncertainties these observables cannot be used for a precise determination of the phase diagram, their discussion is postponed to Sec. 3.8 and chapter 4, respectively.

3.3 Phase Diagram: Development until 1999

In this section, we discuss early results for the fully-frustrated Bethe lattice in high dimensions, i.e., for the homogeneous phase of the Hubbard model with semi-elliptic DOS. The question of how the contrary scenarios of Brinkman and Rice (1970) and Hubbard (1964*b*) for the metal-insulator transition could be be realized in this model was among the first to be attacked numerically after the inception of the DMFT. Rozenberg et al. (1992) pinpointed the Mott-Hubbard transition at $U_\mathrm{c} = 6.2$ for $\beta = 32$ where they observed the disappearance of the quasiparticle peak using QMC.[8] Georges and Krauth (1992) reported $U_\mathrm{c} = 6$ for $\beta = 16$ with an analogous method. A coexistence region of metallic and insulating solutions extending from $U_{\mathrm{c}1} = 5.1$ to $U_{\mathrm{c}2} = 6.6$ at $T = 0$ was found by Georges and Krauth (1993) within iterative perturbation theory (IPT). The more detailed phase diagram by Rozenberg et al. (1994) is shown in two versions: Fig. 3.7 a is taken from the original publication while Fig. 3.7 b is reproduced from the review (Georges et al., 1996). The coexistence region is in good agreement with Georges and Krauth's (1993) earlier estimate. The position of the first-order phase transition line was apparently adjusted in the review on the basis of analytical considerations. The failure of the original IPT scheme to predict the first-order transition line $U_\mathrm{c}(T)$ qualitatively correctly[9] can be linked to the thermodynamic inconsistency of the method which is not a conserving approximation in contrast, e.g., to the DMFT framework itself. As shown in Fig. 3.8 a, the IPT overestimates the double occupancy near the Mott transition (in comparison with ED) at $T = 0$. Thus, the IPT scenario shown in Fig. 3.7 b cannot be quantitatively correct, but should overestimate $U_{\mathrm{c}1}$ and $U_{\mathrm{c}2}$. Otherwise, the IPT phase diagram Fig. 3.7 b, supported by QMC data as shown in Fig. 3.8 b, was considered authoritative.[10]

In fact, it stood until 1998 when our group (Schlipf, 1998) surprisingly could not stabilize a metallic phase in QMC calculations for the presumed coexistence region

[8] In his pioneering DMFT-QMC study, Jarrell (1992) demonstrated Mott-Hubbard behavior, i.e., a vanishing quasiparticle peak and the development of a pseudogap for the hypercubic lattice. The focus of that work, however, was on antiferromagnetism and on the exclusion of superconductivity.

[9] In this context, Georges et al. (1996) note that *"the free energy within the iterated perturbation theory must be evaluated from a functional that gives the mean-field equations by differentiation, rather than from the one-particle Green's function. This is crucial in order to obey the exact property of a second-order transition"* (at $T = 0$).

[10] In the review, Georges et al. (1996) write: *"Detailed comparisons between the iterated perturbation theory approximation and the QMC method at finite temperature have shown excellent agreement for T/D of the order or $1/50$ or higher. In this region, the iterated perturbation theory phase diagram is quite reliable."*