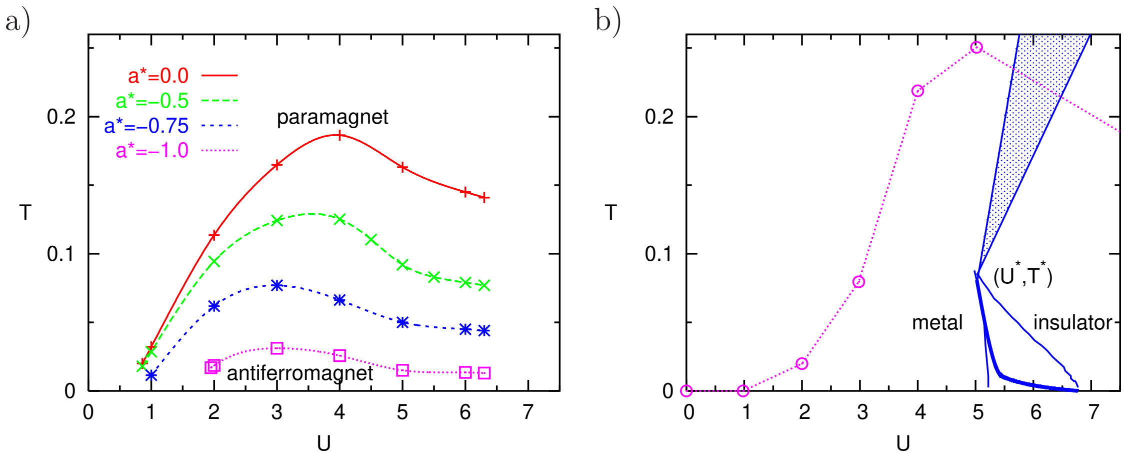

Figure 3.3: Magnetic and MIT phase diagrams for the Hubbard model. **a)** Néel temperature T_{N} for the hc lattice with NN and NNN hopping (Schlipf, 1998). **b)** MIT scenario for the fully frustrated Bethe lattice as computed within IPT (Georges et al., 1996). Here, a first-order phase transition is observed for $T < T^*$ at $U_{\mathrm{c}}(T)$ (thick line) within the coexistence region $U_{\mathrm{c1}}(T) \leq U \leq U_{\mathrm{c2}}(T)$ (thin lines); a crossover region (shaded) extends above T^*. Crosses (connected by a dotted line) indicate T_{N} for the unfrustrated Bethe lattice (Rozenberg et al., 1994); the AF then hides the MIT within IPT.

wide range of interaction strengths $U_{\mathrm{c1}}(T) \leq U \leq U_{\mathrm{c2}}(T)$; the coexistence region (narrow lines) extends up to $T^*_{\mathrm{IPT}} \approx 0.085$.[5] The shaded region at higher temperatures indicates a crossover region.

Schlipf's (1998) QMC calculations of the phase diagram for the hc lattice with NNN hopping showed no traces of a first-order MIT. Even with only NN hopping, no such transition appeared (for a calculation in the homogeneous phase). The contradiction with Rozenberg et al.'s (1995) results was perfect when a first-order MIT line could not even be found for the fully frustrated Bethe lattice at temperatures significantly below the IPT critical temperature (see Sec. 3.3). Thus, new studies became necessary which evolved into a project for this thesis. In this chapter, we will almost exclusively consider the Bethe lattice in the homogeneous phase which is enforced down to $T = 0$. Apart from being relevant on the physical grounds discussed in this section, this model has evolved into a benchmark for the methods of solving the DMFT. Since at least some of the same methods are used for multi-band models and in combination with LDA, the verification of their reliability has consequences far beyond the half-filled single band Hubbard model. The qualitative implications of finite frustration will be discussed in subsection 3.6.4.

[5] Here, energies are scaled to unit variance of the DOS for both models.