Figure 3.2 b shows the resistivity as a function of inverse temperature for various levels of Cr doping. The lowest curve corresponds to the pure case, i.e., the vertical dashed line in the phase diagram Fig. 3.2 a. This curve displays only one kink, a sharp increase of the resistivity by 7 orders of magnitude at the Néel temperature. For sufficiently large doping, a second jump by some 2 or 3 orders of magnitude appears at higher temperature (i.e., going left in the plot) which indicates the Mott metal-insulator transition which is the subject of interest within this chapter.

3.1.2 Theory

A theoretical description of the V_2O_3 phase diagram should at least reproduce its topology including the first-order Mott transition line. If such a description could be found in terms of a purely electronic model, this would be a strong indication for electronic correlations being the driving force behind the Mott transition. Lattice degrees of freedom would, then, appear less important in this respect. While orbital degrees of freedom certainly play an important role for V_2O_3, at least quantitatively [see Held, Keller, Eyert, Vollhardt, and Anisimov (2001) and references therein], the very essence of the Mott transition may already be captured qualitatively by the half-filled single-band Hubbard model. This model is a likely candidate since its paramagnetic phase is a (perfect) metal for $U = 0$ and an insulator for $U = \infty$. A transition would be expected for $U \approx W$ if W is an appropriate measure of the free bandwidth. For the usually considered case of NN hopping on a bipartite lattice, however, the antiferromagnetic phase generically extends to high enough temperatures that the evolution from metal to insulator as a function of U should occur as a smooth crossover. This expectation is indeed an established fact for the Bethe lattice as well as for the hc lattice with NN hopping in infinite dimensions (see below) and is supported by recent QMC results for the simple cubic lattice in $d = 3$ (Staudt, Dzierzawa, and Muramatsu, 2000). Therefore, the Mott transition can only be studied on the Hubbard model when the antiferromagnetic phase is suppressed.

The natural microscopic method of modeling magnetic frustration is the inclusion of hopping terms to (at least) next-nearest neighbors. As discussed in chapter 2, frustration then generically implies an asymmetric DOS. DMFT results for the hypercubic lattice with NN and NNN hopping are shown in Fig. 3.3 a. Here, symbols and interpolating lines indicate the Néel temperature as computed using QMC for an increasing degree of frustration from top to bottom (Schlipf, 1998). Alternatively, antiferromagnetism may be suppressed in analytical and in mean-field methods[4] by restricting solutions to the subspace with appropriate symmetries. For the semi-elliptic Bethe DOS, this choice corresponds, e.g., to solving a fully disordered model where the hopping terms obey $\langle t_{ij}\rangle = 0$ and $\langle t_{ij}^2\rangle = t^{*2}/Z$ (cf. subsection 2.2.2). The phase diagram of this "fully frustrated Bethe lattice" is shown in Fig. 3.3 b as obtained by Georges et al. (1996) within iterated perturbation theory (IPT). According to this result, metallic and insulating solutions coexist at low temperatures over a

[4] Such a suppression is not possible in the context of QMC applied directly in finite dimensions. For this method, the inclusion of NNN is not a practical alternative since it leads to the minus-sign problem. Therefore, finite-dimensional QMC can hardly treat frustration at all.