for the first-order phase transition line based on a scheme using a modified set of self-consistency equations. While the agreement on the level of $U_c(T)$ is impressive, we have found significant discrepancies with respect to the measured double occupancies which this group had used in a Maxwell construction for $U_c(T)$. In addition, we have demonstrated the approximate character of this scheme. We have also studied signatures of critical behavior and have found that its impact on QMC studies is limited to the close surroundings of the (finite-temperature) critical end point of the first-order line. In addition, we have reanalyzed IPT data for the double occupancy in the critical region and have demonstrated that it is governed by a critical exponent of 1/2 rather than the value of 1/3 obtained by Kotliar et al. (2000).

Finally, we have discussed the maximum entropy method (MEM) and its application to the analytic continuation of imaginary-time Green functions computed within QMC. We have demonstrated the strong improvement resulting from our correction of the QMC code and devised a robust MEM scheme that takes the remaining systematic errors into account. By applying this method to large sets of precise QMC measurements, we have calculated the first low-temperature MEM spectra in the MIT region which do not depend on specially chosen ("annealed") default models. The overall high precision of the results is indicated by the good agreement with analytical bounds for the total bandwidth and by the excellent agreement with a sum rule for the derived real-frequency self-energy (to be discussed in Sec. 4.6).

In view of the excellent internal consistency of our results and the good agreement with data obtained using other methods (within their respective error bars), our final phase diagram Fig. 3.50 and other results presented in this chapter should represent a fairly precise and complete picture of the local properties of the fully frustrated model. However, they clearly do not represent a complete scenario for any material featuring a MIT. This follows already from the finite ground-state entropy predicted in the insulating phase which violates Nernst's law. A more realistic and consistent description is possible when the low-temperature phase is ordered already in $d = \infty$, i.e., for partial frustration. Analytical considerations for the consequences in the case of varying partial frustration at constant semi-elliptic DOS have been presented in this chapter. Investigations whether a phase diagram with a topology analogous to that seen in V_2O_3 can also be observed in the generic case that frustration induces an asymmetry of the DOS have recently been initiated under our supervision (Knecht, 2002); at present, this question is still open.

A further significant improvement of the QMC code based on ideas developed in this thesis and implemented by Knecht (2002) is briefly discussed in App. C; numerical comparisons shown in this appendix also demonstrate the high accuracy of the (less general) approach employed within this work. Future DMFT studies could also greatly profit from a scheme for the direct evaluation of differences in the free energy of coexisting solutions developed in this chapter.