the QMC hysteresis runs were performed at constant temperature. The interpolating line is a guide to the eye only; it is certainly compatible with the $T = 0$ estimates for U_{c2} by ED and PSCT (Moeller, Si, Kotliar, Rozenberg, and Fisher, 1995). Still, the scenario of a continuous transition is in fundamental qualitative disagreement with both ED (squares in Fig. 3.9 indicate the zero-temperature results, note the large error bars) and IPT.

Our controversial result stirred new interest in the problem. Qualitatively, the continuous scenario was supported by results from the random-dispersion approximation (RDA), evaluated using ED on a small cluster. Quantitatively, however, the agreement was hardly better than, e.g., with IPT, since the (zero-temperature) RDA result of $U_c = 4$ (shown as a circle in Fig. 3.9) is clearly too small to be compatible with the QMC data.

The result of a new QMC study by Rozenberg, Chitra, and Kotliar (1999), in contrast, was quantitatively almost compatible with our data (within double error bars[12]). It also confirmed that the QMC coexistence point computed earlier by Rozenberg et al. (1994) and shown as triangle in Fig. 3.9 was indeed incorrect. However, the new study demonstrated the coexistence of metallic and insulating solutions (triangles in Fig. 3.10) in a temperature range where Schlipf et al. (1999) had ruled out a first-order transition. Further support for the scenario of a first order transition came from zero-temperature NRG studies (Bulla, 1999). The resolution of this contradiction, obtained for the same model (and now even using the same numerical methods) became an important project for this thesis and will be the subject of the remainder of this chapter. The first part, the verification of coexistence, was accomplished in the fall of 1999, soon after Rozenberg made available a set of QMC estimates for $G(\tau)$ and $\mathcal{G}(\tau)$ in both the metallic and insulating phase for the single parameter set $T = 1/32$, $U = 4.92$ (cf. Fig. 3.12).[13] At this point, all involved groups accepted that a finite, but small coexistence region was established in the lowest temperature range studied so far using QMC. Still, the shapes of the coexistence region were unclear. The thick solid lines in Fig. 3.10 represent Kotliar's perception that the region should broaden significantly for lower T, reaching the RDA point for U_{c1} and matching the (practically identical) estimates for U_{c2} obtained using ED, PSCT, and NRG (see Table 3.1 on page 112).

3.4 Discussion of QMC Algorithms

In the main part of this section, we will discuss two aspects of the quantum Monte Carlo (QMC) algorithm for the DMFT self-consistency problem: the discrete Fourier transformations between imaginary time and Matsubara frequencies and the search strategy for solutions of the DMFT equations. Both aspects are directly relevant for the detection of the Mott transition and the associated coexistence region. The different algorithms for handling the discrete Fourier transform used in the codes

[12] The point at $T = 1/30$ with the small error bar was not computed as part of this thesis.

[13] Note that this phase point is not among the previously published data, but more in the center of the claimed coexistence region.