continuum limit is recovered for $\tilde{\Lambda} \to 1$. Attributing the differences between NRG and QMC to the known systematic underestimation of critical interactions by NRG at large $\tilde{\Lambda}$ (and finite temperature), the agreement appeared reasonable, in particular when compared with IPT (thin lines).

Figure 3.32 b represents the status of the phase diagram of late October 2000.[29] Here, our QMC estimates (crosses) are already based on measurements of the full internal energy (cf. subsection 3.5.1). This fact and a large number of simulations on a finer grid result in an accuracy which is much higher than that of the preliminary results shown in Fig. 3.32 a and also significantly higher than that of Joo and Oudovenko's (2001) results shown as squares in Fig. 3.32 b (which were first available as preprints in late September 2000).[30] The surprisingly good agreement between our QMC results and the improved NRG results [which are close to, but not identical with the data shown in the subsequent publication (Bulla et al., 2001)] is partially accidental as the final results for QMC and NRG show slightly larger differences (cf. subsection 3.6.3). Still, the good overall agreement between these results and (within larger error bars) with the independent QMC results obtained by Joo and Oudovenko (2001) indicated a resolution of the controversy towards a reliable phase diagram. In particular, the improved NRG estimate $U_{c2}(T=0) = 5.86$ is practically identical with the PSCT/ED estimate $U_{c2}(T=0) = 5.84$. These and all other published numerical estimates for the boundaries of the MIT coexistence region at $T=0$ that we are aware of are reproduced in Table 3.1. A corresponding summary for the coordinates of the second-order critical end point is given in Table 3.2; the latter also includes our new QMC estimate.

The thick line in Fig. 3.32 b which evolves into a dashed line at low temperatures reflects our estimate (as of October 2000) of the true first-order phase transition line; the final estimate (which is hardly distinguishable from the curve shown here) will be presented after detailing the methodology in Sec. 3.6. The low-temperature part of this curve is partially based on the assumption that $U_{c2}(T=0) \approx 5.85$ which is certainly justified based on the excellent agreement between PSCT, ED, and NRG.

Leaving the historical review, let us discuss the possible origin of the remaining discrepancies between the various QMC estimates of the boundaries of the coexistence region. Tilted and upright crosses in Fig. 3.33 represent our extrapolated QMC data (here repeated from Fig. 3.31) and QMC data corresponding to $\Delta\tau = 0.25$, respectively. Evidently, the extrapolation $\Delta\tau \to 0$ is important; otherwise (i.e., at $\Delta\tau = 0.25$), the coexistence region is shifted by about $\Delta U \approx 0.1$ towards larger interaction and by about $\Delta T \approx 0.005$ towards higher temperatures.[31] Interestingly,

[29]The comparison shown here was prepared for a conference in Grenoble (starting on October 30, 2000); on that occasion, a paper copy was also handed out to Georges. The same data (including our estimate for the first-order phase transition line) was presented in talks in condensed matter theory seminars in Augsburg and Mainz on 11/29/00 and 12/05/00, respectively and appeared in a report sent to the van Neumann Institute for Computing in November 2000.

[30]Note that Joo and Oudovenko (2001) did not calculate the tip of the coexistence region. Instead, they used Rozenberg et al.'s (1999) earlier estimate.

[31]Note that in our computations, the range of discretization parameters includes $0.1 \leq \Delta\tau \leq 0.25$ even for relatively low temperatures $T \geq 0.025$ ($\Delta\tau_{\text{min}} = 0.125$ for $T = 0.02$). Therefore, the deviation of our best "raw" results from the extrapolated results is much smaller than shown in this