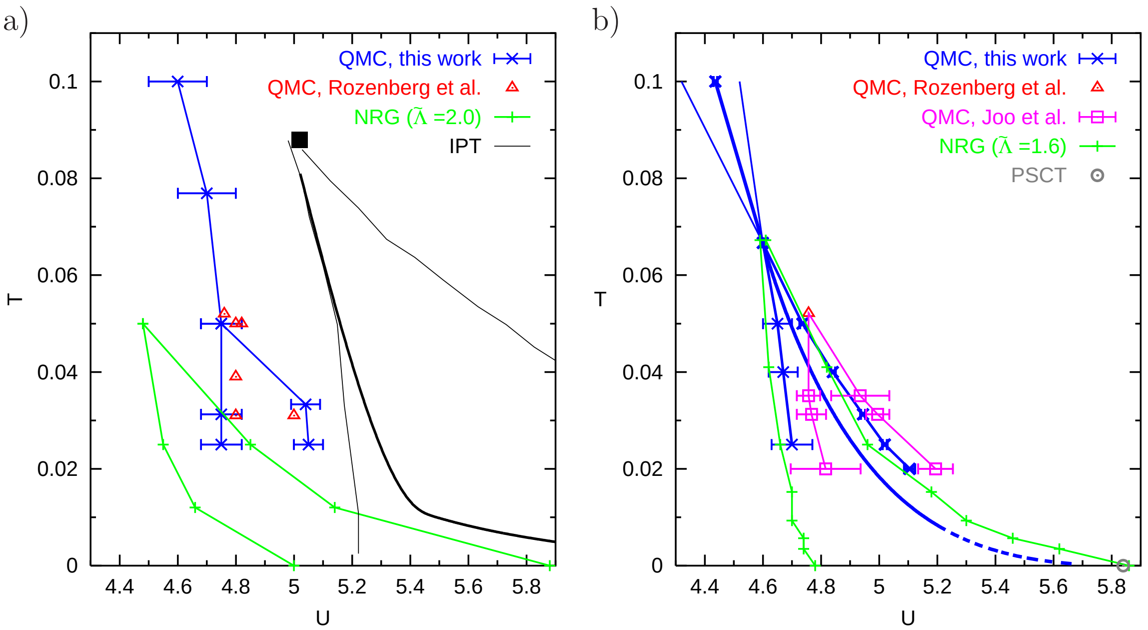

Figure 3.32: MIT phase diagram: **a)** Status as of Spring 2000 as established by this work, Rozenberg et al. (1999), and by preliminary NRG results for discretization $\tilde{\Lambda} = 2.0$ (Bulla, unpublished) in comparison with the IPT scenario [Georges et al. (1996); cf. Fig. 3.7]. **b)** Status as of Fall 2000: improved QMC estimates (this work), preliminary NRG results for discretization $\tilde{\Lambda} = 1.6$ (Bulla, unpublished), and new QMC boundaries by Joo and Oudovenko (2001) which include the critical point determined by Rozenberg. The NRG estimate for $U_{c2}(T = 0)$ is in excellent agreement with PSCT (Moeller et al., 1995).

green tilted rectangle. A reasonable numeric representation is $\Delta T = 0.004$, $\Delta U \lesssim 0.03$. The coexistence region shown in Fig. 3.31 is one of the main results of this thesis: It resolves the dispute described in subsection 3.1.2 and Sec. 3.3 since it essentially confirms Rozenberg et al.'s (1999) earlier and Joo and Oudovenko's (2001) independent QMC results and shows excellent agreement with independent NRG results (Bulla, Costi, and Vollhardt, 2001). In addition, our result has the smallest errors.

Before we further substantiate these claims, let us take a short look at the historical development. The tilted crosses in Fig. 3.32 a represent early QMC results obtained using the corrected code (cf. subsection 3.4.1) as presented at the DPG spring meeting on March 30, 2000. Here, lines are guides to the eye only. Within their (large) error bars, these preliminary results for the boundaries of the coexistence region were fully consistent with the coexistence points (triangles) previously found by Rozenberg et al. (1999). At the time of the conference, finite-temperature NRG estimates (Bulla, unpublished[28]) were not yet reliable: the horizontal crosses in Fig. 3.32 a correspond to an energy discretization parameter $\tilde{\Lambda} = 2.0$, where the spectrum is modeled by a discrete set of δ-peaks at energies $\pm E_0 \tilde{\Lambda}^n$; the physical

[28] The NRG points at $T = 0$ coincide with previously published data (Bulla, 1999).