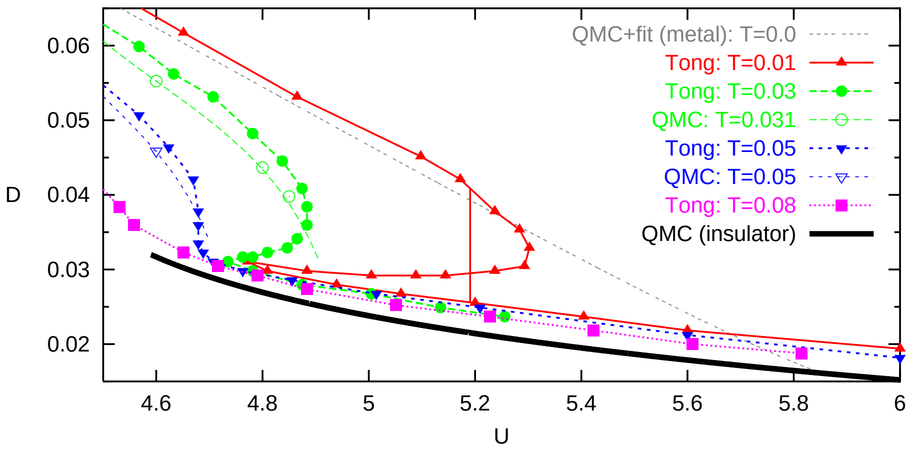

Figure 3.53: Double occupancy: Full symbols connected by thick lines represent results obtained using the approximate transformation technique (Tong et al., 2001). The non-unique part of the curves for $T \leq 0.05$ is interpreted as a set of metallic, unstable, and insulating solutions (from top to bottom). The first-order transition can be pinpointed by using a Maxwell-construction which includes the unstable solution (vertical line at $U \approx 5.2$ for $T = 0.01$). Empty symbols and thinner lines show the QMC results for the metallic phase; the thick black line shows the QMC result for the insulating phase (cf. Fig. 3.42).

scenario shown in Fig. 3.53 is plausible, provided that a third solution of the DMFT equations exists. Then, the knowledge of the approximate shape should suffice for a reasonably accurate estimate for $U_c(T)$ within the range spanned by $U_{c1}(T)$ and $U_{c2}(T)$. An even more direct method for the comparison of free energies will be proposed in subsection 3.7.2.

Figure 3.54 shows a comprehensive comparison of results for the MIT in the half-filled fully frustrated Hubbard model with semi-elliptic DOS in $d = \infty$. One important point that should be conveyed by this (admittedly somewhat busy) figure is the convergence of recent estimates for the boundaries U_{c1} and U_{c2} of the coexistence region and the significant improvement over old IPT and QMC results. Thus, the controversy stirred by Schlipf et al.'s (1999) paper has lead to secured knowledge of the properties of this model with unprecedented accuracy. Among the more recent results, those obtained by Joo and Oudovenko (2001) are least precise; in fact, their estimates for U_{c2} are above upper bounds established in this work (cf. Fig. 3.31 and Fig. 3.32 b). Low-temperature information is only provided by Bulla et al. (2001) and Tong et al. (2001) with apparently about equal precision; the agreement with our QMC data for $T \leq 0.025$ is excellent. The origin of the discrepancy between NRG and the other methods near the tip of the coexistence region at $T \approx 0.05$ is unclear; possibly, the systematic NRG error (due to the finite energy discretization $\tilde{\Lambda} = 1.6$) is most significant in this temperature range. Still, the available data clearly supports the high accuracy of our QMC results.

A second point of hardly minor importance is that no qualitatively correct prediction for the first-order transition line preceded our first estimate (cf. Fig. 3.32 b);