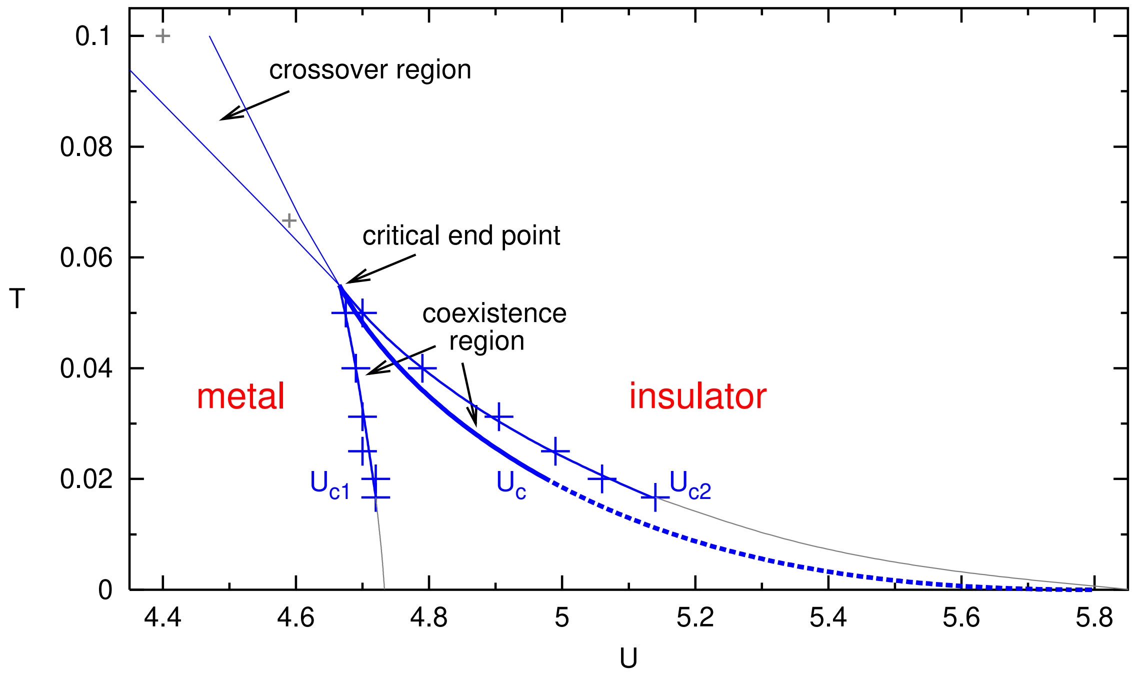

Figure 3.50: Final MIT phase diagram: Above the critical point (with coordinates $U^* = 4.665$ and $T^* = 0.055$), increasing interaction U causes a smooth transition from a metal towards an insulator; the change is most rapid within the crossover region. For $T < T^*$, the metallic phase is thermodynamically stable for $U \leq U_c$, but remains a well-defined metastable solution of the DMFT equations for $U_c < U \leq U_{c2}$. Conversely, a well-defined insulating phase solves the DMFT equations for $U \geq U_{c1}$, but is thermodynamically stable only for $U \geq U_c$. The QMC data (crosses) and thin blue lines are identical to Fig. 3.31. The thick blue line (partly dashed) represents the QMC result for $U_c(T)$ obtained in this section. Faint grey lines extrapolate the QMC data for U_{c1} and U_{c2} to $T = 0$.

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for $U \to U_c^0$. The agreement with $T = 0$ NRG data is reasonable. Note that the curvature of $\gamma^{-1}(U)$ has to be large near U_c^0 in order to reconcile the data in the range $U < 5.2$ with a value of $U_c^0 \approx 5.85$. Therefore, the slope near U_c^0 is necessarily much smaller than at lower $U \lesssim 5.2$. Still, the NRG predictions near U_c^0 seem a bit low, in particular when interpreted in terms of $\gamma^{-1}(U)$ which might explain the remaining discrepancy in comparison to our linear fit. So our results have indeed passed a nontrivial test.

While our method of determining the position of the first-order phase transition line on the basis of QMC data represents the first serious successful attempt of a controlled comparison of free energies for Hubbard-like systems, the first publication of a quantitatively correct result for $U_c(T)$ is due to Tong et al. (2001). Their results for U_{c1}, U_c, and U_{c2}, shown as circles in Fig. 3.52 became publicly known (as preprint) in late May 2001, about half a year after our first results had been presented (cf. footnote 29 on page 111). With the exception of our lower estimates for $U_{c1}(T)$, the agreement with our final QMC results (crosses and blue lines) appears nearly