Generally, the solution of a linear differential equation can be written as a regular integral. Specifying the initial condition as $U_c(T=0) = U_c^0$, we have here

$$U_c(T) = e^{43T}\left(U_c^0 + \int_0^T dT' e^{-43T'} A(T')\right). \tag{3.51}$$

With $A(T)$ given by (3.49) and the parameters stated above, this integral can even be performed analytically. Since the derivation is both lengthy and straightforward, it is omitted here. Adjusting the initial condition so that the solution goes through the tip of the coexistence region leads to $U_c^0 \approx 5.795$. This value is smaller than the value $U_c^0 \approx 5.85$ obtained from PSCT, NRG, and ED and used in our ground state fits for E and D. In our view, the observed discrepancies reflect the limits of the linear approximation for the dependency of $f(T,U)$ on U. While deviations from the linear form are small within the coexistence region, i.e., in the range $4.7 \lesssim U \lesssim 5.0$, this need not be the case for $U \to U_c^0$. Still, the deviation of about 6% (if measured from the last direct QMC data point at $U \approx 5$) is surprisingly small considering the various potential sources of errors.[44]

The full phase diagram of the half-filled Hubbard model with semi-elliptic DOS in $d \to \infty$, the main result of this chapter, is shown in Fig. 3.50. Here, crosses and thin lines indicate the boundaries of the crossover and coexistence region as already seen in Fig. 3.31. The true thermodynamic first-order phase transition line computed in this section, i.e., the solution of (3.51) for the fit defined by (3.49) and (3.50) is drawn as a thick line in Fig. 3.50. It is fully based on QMC data at least in the range $T \geq 0.02$ where direct QMC estimates for $f(T,U)$ are available. The dashed line style used below this range is a reminder that the PSCT/ED/NRG estimate of $U_c^0 \approx 5.85$ was used at some stage of the derivation of the low-temperature form of $U_c(T)$. The various numerical checks performed on the basis of extrapolated QMC data suggest, however, that the impact of possible errors in this external input on our final result is minimal.

A final test of consistency can be performed on the basis of the full solution $U_c(T)$ by computing an additional term in its low-temperature asymptotics. Then, (3.37) is refined as

$$U_c(T) = U_c^0 - \sqrt{\frac{2S_o T}{a}} + \frac{\gamma_0}{4S_0} T + \mathcal{O}(T^{3/2}), \tag{3.52}$$

where all symbols are known from subsection 3.6.2. Thus, the linear coefficient of $U_c(T)$ can be compared with asymptotic ground state results for the linear coefficient of the specific heat $\gamma(U)$ and [using $\gamma = 2\pi/(3Z)$] also with ground-state estimates of the quasiparticle weight Z. This comparison is shown in Fig. 3.51. In Fig. 3.51 a, the coefficients of the contributions of order T and $T^{3/2}$ to $U_c(T)$ are determined as 28 and -100, respectively. Consequently, consistency demands that $\gamma(U) \approx 72/(U_c^0 - U)$

[44] An even better agreement at small T could have been achieved by using a larger leading coefficient of the square-root divergence in $A(T)$, i.e., a smaller value of a. The latter would be consistent with the results of our QMC extrapolations to $T=0$ if the curvature of the double occupancy was strongly enhanced near U_c^0. Such behavior is certainly possible as seen in the NRG curve for $Z(U)$ in Fig. 3.48.