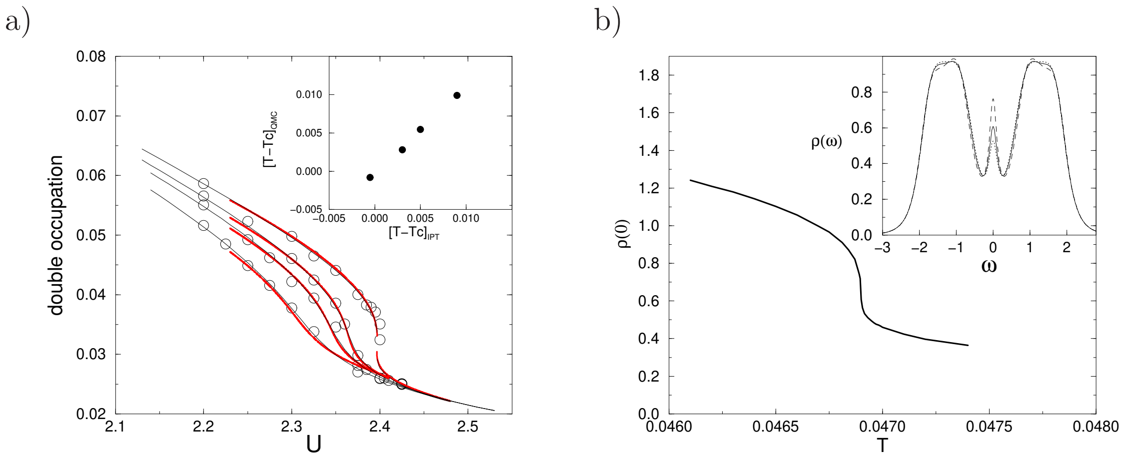

Figure 3.59: a) Double occupancy versus U for T slightly below (top set or curves/symbols) or above T^* (lower 3 data sets, with increasing T towards the bottom) as estimated from QMC (circles) and IPT (thin lines). Thick lines represent fits according to the Ginzburg-Landau theory. **b)** IPT density of states at the Fermi level versus T for $U = 2.46316 \approx U^*_{\mathrm{IPT}}$. The insets are irrelevant for our discussion. Both figures are reproduced from the publication by Kotliar et al. (2000). Energies are in units of the half bandwidth.

---

so that the corresponding susceptibility $\chi = \partial D/\partial U$ diverges as $|U - U^*|^{-2/3}$ for $T = T^*$. In the following, we will show that the IPT data and (rescaled) QMC data presented in the cited paper fail to support this claim.

In order to simplify the discussion, we have reproduced both figures of the cited paper as Fig. 3.59. In the main panel of Fig. 3.59 a, QMC estimates for the double occupancy D (circles) for the temperatures $T = 1/40$, $T = 1/35$, $T = 1/32$, and $T = 1/25$ (from top to bottom) have been scaled on IPT estimates (thin lines) for the temperatures $T = 0.0469$, $T = 0.05$, $T = 0.052$, and $T = 0.056$; here, all energies are measured in units of the half bandwidth and have to be doubled to correspond to the units used throughout the rest of this chapter. Thick lines show fits derived from the Ginzburg-Landau theory. Evidently, the only candidate for singular behavior among these data sets is that for the lowest temperature(s); a magnified view on this data is given in Fig. 3.60. Here, the QMC results (circles) are connected by lines to guide the eye. Note that the two QMC data points at $U \approx 2.40$ have been computed for the same interaction; consequently, they imply coexistence rather than a diverging slope of the metallic solution. For enhanced clarity, the IPT data is shown as crosses (instead of a thin line) in Fig. 3.60. In addition to the Ginzburg-Landau (GL) fit (solid line), we have added a pure cubic-root fit of the form $D(U) = 0.0305 + 0.035 * (2.3974 - U)^{1/3}$ for the metallic phase.[51] A first

[51] While the technique employed here for extracting the data from the postscript figures (available from the preprint archive) is exact for relative positions of symbols and line segments, a slight mismatch in overall scale and offset is in general unavoidable.